



Chemical Insights into Psoriasis Drugs via Entropy and Quantitative Structure-Property Relationship Analysis for the Applications of Environmental Nanotechnology

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ABSTRACT

Pharmaceutical residues released into aquatic and environmental systems are emerging contaminants of concern, creating a need for efficient computational approaches to characterize their molecular properties and support environmental assessment. This study investigates ten commonly prescribed drugs used in psoriasis treatment through degree-based topological indices and entropy measures within a quantitative structure–property relationship (QSPR) framework. The molecular structures of the selected pharmaceuticals were represented as molecular graphs, and degree-based entropy descriptors were calculated to quantify structural connectivity, molecular complexity and information content. Linear, quadratic, cubic and logarithmic regression models were developed to examine the relationships between these descriptors and selected physicochemical properties relevant to the environmental behaviour and molecular characterization of pharmaceutical compounds. The results demonstrate meaningful associations between several degree-based entropy measures and the investigated physicochemical properties, while cubic regression models generally exhibited improved predictive performance for several properties. The findings highlight the potential of graph-theoretical and entropy-based descriptors as computational tools for predicting molecular characteristics of pharmaceutical contaminants. Such approaches can contribute to preliminary environmental risk assessment, contaminant characterization and the rational evaluation of pharmaceutical molecules relevant to advanced environmental monitoring and nano-enabled remediation strategies. The study demonstrates how molecular graph descriptors can complement conventional approaches for computational assessment of emerging pharmaceutical contaminants in environmental systems

Keywords: Psoriasis drugs; Environmental technology; Anti-inflammatory; Skin; Entropy; Nano-enabled materials.

1. INTRODUCTION

Psoriasis is a inflammatory skin disorder that affects quality of life and may involve both skin and joints. Its management requires therapeutic agents with chemical structures and physicochemical characteristics. Understanding the molecular features of these compounds is therefore important for comparison and computational assessment. Conventional experimental characterization of every candidate can be time consuming and intensive, creating a need for computational approaches that can extract effective information directly from molecular structure. In this context, graph-based methods provide a representation of chemical systems and can support analysis of molecular connectivity and complexity. Such approaches are particularly useful when structural information must be converted into descriptors for statistical modelling. The physicochemical behaviour of a drug is influenced by its molecular architecture, and descriptors derived from molecular graphs can provide a compact means of capturing structural differences among related compounds (Henseler and Christophers, 1995; Griffiths

and Barker, 2007; Kamiya et al. 2019; Elder et al. 1994; Armstrong and Read, 2020). Graph theory offers a framework for representing chemical structures through vertices and edges. In a molecular graph, atoms are represented by vertices and chemical bonds by edges, allowing structural connectivity to be analysed mathematically. Topological indices derived from these graphs have been widely investigated as descriptors of molecular structure and have applications in chemistry, materials science, toxicology, bioinformatics and drug development (Menter and Griffiths, 2007). Entropy measures provide an way of quantifying structural diversity or complexity within graph representations. The combination of topological indices and entropy can therefore provide descriptors that reflect differences in molecular organization and connectivity. This computational perspective is relevant to molecular and nanostructure modelling, where graph representations are used to characterize complex chemical networks and structural architectures (Koam et al. 2023). Quantitative structure-property relationship (QSPR) analysis uses mathematical relationships between molecular descriptors and physicochemical properties to develop

predictive models. By relating topological and entropy descriptors to measurable properties, QSPR can reduce the dependence on extensive preliminary experimental screening and help identify descriptors with useful predictive capability. The present work applies degree-based entropy descriptors to ten drugs used for psoriasis and evaluates their relationships with physicochemical properties. Linear, quadratic, cubic and logarithmic regression models are compared to determine which mathematical forms provide the effective predictions. The study therefore combines chemical graph theory, entropy-based molecular characterization and QSPR modelling in a computational framework. Beyond the immediate pharmaceutical application, the approach demonstrates how structure-derived descriptors can be used for quantitative chemical characterization and may support computational studies of molecular systems, including chemically complex and nano-enabled materials. The objective is to establish interpretable relationships between molecular structure and physicochemical behaviour while identifying regression models that provide reliable predictive performance. The selected compounds include methotrexate, leucovorin, cyclosporine, adalimumab, retinoid, anthralin, salicylic acid, cefaclor, apremilast and tazarotene, representing therapeutic molecules. Their molecular graphs provide a basis for calculating degree-based indices and entropy values. The resulting descriptors are examined against properties such as boiling point, flash point, enthalpy of vaporization, molar refractivity, polarizability, molecular volume, molecular weight and parameters. Comparing several regression forms allows the predictive behaviour of different descriptors to be evaluated rather than relying on a single statistical relationship. This is important for identifying descriptors that capture meaningful structural information and for improving the interpretability of QSPR models. Accordingly, the study emphasizes a computational route for connecting molecular topology, entropy and physicochemical behaviour. Descriptor-based approaches can complement experimental research by prioritizing molecules for further characterization and comparing structurally different compounds quantitatively.

2. RESEARCH AIMS

In order to predict the chemical structure of ten frequently given medications for psoriasis, this study uses degree based entropies, a comparatively unexplored field in QSPR analysis. The article aims to fill a significant gap in the literature by concentrating on psoriasis and offering insights in order to improve drug design. Quantitative structure property relationship models generate prediction models from datasets for corresponding physicochemical properties using a variety of computational techniques, like curvilinear regression analysis. By offering trustworthy predictions regarding the behavior of untested molecules, QSPR

aims to decrease the time and expenses related to experimental testing. Topological indices are the most main descriptors utilized in QSPR analysis. These indices, which are numerical values obtained from molecular graph, provide details on its structural characteristics and connectivity. These indices are widely used in many different fields, including materials science, toxicology and drug development. This work offers a more thorough analysis of QSPR techniques and the function of entropies in forecasting biological activities. Using TIs, scientists have been using the QSPR and QSAR methodology more and more in recent years to forecast the physicochemical characteristics or biological activity of chemical compounds. (Kirmani *et al.* 2021) utilized TI for exploring the QSPR of analgesics drugs of COVID-19. (Gnanaraj *et al.* 2023) investigated the properties of NASID pharmaceuticals. The QSPR modeling technique has versatile predictive ability in discovery of drugs. (Zhou *et al.* 2024) used the QSPR model to investigate the thermodynamic properties of narcotic medications. (Zaman *et al.* 2024) found models of novel drugs applied in blood cancer treatment. (Nasir, 2025) used QSPR modelling in colorectal disease and demonstrated that QSPR technique is most effective in predicting the properties of medications and also yields valuable results about blood cancer (Nasir *et al.* 2022). Researchers were inspired to use QSPR approaches by flexible analysis of medications for schizophrenia (Zhang *et al.* 2023; Farooq *et al.* 2023) conducted QSPR modelling and examined the topological indices of novel HIV medications. The indicators associated with Kulli Nirmala strongly suggest or project a sense of superiority of these indices (Kulli *et al.* 2021; Sultana, 2023) used QSPR to find the chemical uses of topological markers in creating medications to cure infertility. (Farooq *et al.* 2022) conducted a work on implication of TIs on QSPR modeling of drugs. The work on QSPR modeling has been thoroughly utilized and implemented in a well-versed manner (Awan *et al.* 2024).

Malaria remains a fatal disease worldwide. Modeling of drugs for malaria when conducted, yielded highly correlated and reliable models. To evaluate the physicochemical characteristics of potential antimalarial drugs, (Awan *et al.* 2025) employed topological indices in a QSPR analysis and developed QSPR models that proved effective for babesiosis drugs. Similarly, (Koam *et al.* 2023) investigated the entropy properties of nanotubes. Several studies have been conducted on the use of TIs in QSPR analyses of various medications. (Imran *et al.* 2019) investigated the topological indices of dendrimers. Graph-theoretical results for a diverse range of drugs have been reported by (Wei *et al.* 2024; Abubakar *et al.* 2024) used machine learning models and showed effective QSPR models in drugs discovery.

The purpose of this study is to examine the degree-based entropy of frequently prescribed medications for psoriasis. The urgent need for efficient

therapies and the ability of computational techniques to forecast physicochemical characteristics without requiring lengthy laboratory testing serve as the driving forces. This study opens the door for further developments in medicinal chemistry by demonstrating the value of degree-based entropies in comprehending the connection between chemical structure and therapeutic characteristics for psoriasis. The drugs shown in Fig. 1 are examined using QSPR modelling to determine their efficacy and suitability for treating this condition:

- Methotrexate is an antineoplastic agent used in the treatment of a wide variety of cancers as well as severe psoriasis, severe rheumatoid arthritis and juvenile rheumatoid arthritis.
- Apremilast is a non-steroidal drug used for the treatment of inflammatory conditions such as psoriasis and psoriatic arthritis.
- Cyclosporine is a steroid-sparing immunosuppressant used in organ and bone marrow transplants as well as inflammatory conditions such as ulcerative colitis, rheumatoid arthritis, and atopic dermatitis.
- Adalimumab is a monoclonal anti-tumor necrosis factor alpha antibody used in the treatment of a wide variety of inflammatory conditions such as rheumatoid arthritis, Crohn's disease and ankylosing spondylitis.
- Retinoid is a group of chemical compounds derived from or related to vitamin A. They are used in skincare to treat various conditions, including acne, wrinkles, and psoriasis. Retinoids work by interacting with retinoic acid receptors which influence cell growth and differentiation.
- Anthralin is an anthracene used to treat stable plaque psoriasis.
- Salicylic acid is used to treat acne, psoriasis, calluses, corns, keratosis pilaris.
- Leucovorin is a folate analog used to treat the toxic effects of methotrexate and other folate antagonists, to treat megaloblastic anemia, and to provide palliative treatment of cancer.
- Tazarotene is an acetylenic retinoid used to treat fine wrinkles, mottled pigmentation of the skin, acne vulgaris, and plaque psoriasis.

For psoriasis and its consequences to be adequately managed, these medications are necessary. These medications were chosen because of their widespread use in clinical settings, efficient modes of action, low incidence of adverse effects, demonstrated effectiveness in combination treatments, accessibility and cost and robust clinical data backing them up. To ascertain the degree-based entropies, visual representations of the drug structures have been created (Fig. 2) and used computational techniques as well as vertex and edge splitting methods. To accelerate the calculations and data processing, an algorithm supported computerized calculating technique was used by implementing MatLab. The degree-based entropies of drugs in Table 1. Using SPSS software, we used various regression models and looked into the QSPR analysis of the computed indices, as shown in Table 2 to Table 14. A number of properties, such as boiling point (BP), flash point (FP), enthalpy of vaporization (E), polarizability (P) etc., have demonstrated high predictive potential when modelled using particular entropies. R-language was implemented (version 2022) in to speed up the entropy computation.

2.1 Significance of This Work

Novel topological index entropies are computed for psoriasis drugs and their physicochemical properties are used to do QSPR analysis and successfully analyzed.

- While most research uses linear regression models, this study is different in that it extends the regression models for cubic and quadratic, logarithmic, exponential and multiple forms for improved efficacy.
- In order to analyze the physicochemical characteristics of the medications under consideration, a number of statistical parameters are calculated and compared with the degree-based entropies.
- Graphical comparison of regression models is also done.

3. MATERIAL AND METHODS

3.1 Topological Indices and Entropy Measurement

Topology index is a simple yet powerful tool for understanding molecular behavior. This supports researchers in environmental chemistry, material science and drug development by enabling them to find novel

medications and produce molecules with specific qualities. The current research in the development and application of topological indices is an important factor in the advancement of computational chemistry and molecular modelling.

In this scenario, by measuring entropy, one can determine the structural diversity or complexity of chemical compounds depicted as graphs. The Shannon entropy is a commonly used entropy measure that is calculated using the distribution of particular structural features within a set of chemical graphs. In addition to topological features like connection patterns and Shannon entropy can be computed from the distribution of atom and bond types. A higher entropy number indicates greater diversity or variability in specific structural features within the set of molecules. Entropy in Y-junction nanostructures was investigated by (Koam *et al.* 2023; Chen *et al.* 2014) introduced the concepts of entropy in edge-weighted graphs. In Eq. (1), the entropy of an edge-weighted graph is given.

$$ENT_Y(G) = - \sum_{\theta, \kappa \in E(G)} \frac{Y(\theta, \kappa)}{\sum_{\theta, \kappa \in E(G)} Y(\theta, \kappa)} \log \left[\frac{Y(\theta, \kappa)}{\sum_{\theta, \kappa \in E(G)} Y(\theta, \kappa)} \right] \quad \dots (1)$$

The topological index functions for A1, A2, A3, A4, A5, A6, A7, A8, A9, A10, A11 and A12 along with their entropy indices are provided in Table 1. In this paper, we focus on psoriasis drugs such as methotrexate, leucovorin, cyclosporine, adalimumab, retinoid, anthralin, salicylic acid, cefaclor, apremilast and tazarotene. The molecular structures of these drugs are displayed in Fig. 1. Here the author mentions the technique to utilize the Table 1 formulas to obtain the results of the following sections. Table 2 shows the degree-based entropies for ten psoriasis drugs calculated using Eq. (1) and R-language. We now explain the computation of degree-based indices for the $BM(G)$ index through edge partitions by considering methotrexate (a) as the reference structure. The methotrexate edge partition of E (1,3), E (2,3), E (2,2) and E (3,3) are 8,18,4,5. By inserting these values in the formula for $BM(G)$ we get:

$$BM(G) = 8[(1 + 3) + 1 \times 3] + 4[(2 + 2) + 2 \times 2] + 18[(2 + 3) + 2 \times 3] + 5[(3 + 3) + 3 \times 3] = 361$$

Now, by using indices from equations (10) to (17) in formulae of entropy, given in Table 2, we obtain the entropy of Bi-Zagreb $ENT_{BM}(G)$ index is:

$$ENT_{BM}(G) = \log(361) - \frac{1}{361} \log [(8)(1 + 3 + 1 \times 3)^{(1+3+1 \times 3)} \times (4)(2 + 2 + 2 \times 2)^{(2+2+2 \times 2)}]$$

$$\begin{aligned} &\times (18)(2 + 3 + 2 \times 3)^{(2+3+2 \times 3)} \times \\ &(5)(3 + 3 + 3 \times 3)^{(3+3+3 \times 3)}] \\ &= 2.43 \end{aligned}$$

On applying same technique with formulas on other drugs, the Table 2 calculation can be done with appropriate software like R-language

3.2 Curvilinear Regression Analysis of Psoriasis Drugs

This section provides an overview of different regression equations.

- (i) $P = a \ln(p_1)$ (Logarithmic Equation)
- (ii) $P = a + k_1 p_1$ (Linear Equation)
- (iii) $P = a + k_1 p_1 + k_2 p_1^2$ (Quadratic Equation)
- (iv) $P = a + k_1 p_1 + k_2 p_2^2 + k_3 p_3^3$ (Cubic Equation)

In this study, a regression model (RM) with coefficients p_1 , p_2 and p_3 were used to analyse the entropy (X) and physicochemical property (P). In addition, the correlation coefficient (F) and the number of samples (n) were taken into account (Zhang *et al.* 2023). The physicochemical property values were the dependent variable in the linear, quadratic, cubic and logarithmic regression models, whilst the TIs were the independent variables. The correlation coefficient (R) statistic was used to assess the model's predictive power; the model with the lowest error was deemed to be the best. Regression analysis, forecasting, and climatology all frequently utilize RMSE to evaluate how accurate experimental results are. For example, if all of the points fall on the regression line, indicating no errors, the RMSE value will be zero if the correlation coefficient is 1. The predictive power of the model is assessed using the RMSE measure, and the best model is one with the least amount of error (Armstrong and Read, 2020). The maximum R², R, F, and least standard error values were used to identify the optimal model.

4. DISCUSSION AND ANALYSIS OF QSPR MODELS

Eleven physicochemical properties of drugs found at <https://pubchem.ncbi.nlm.nih.gov/> were used to analyze psoriasis. Tables 1 and 2 present the degree-based entropies. A two-dimensional linear visualization comparing different entropies is shown in Fig. 1. The correlation coefficients (R) between the degree-based

entropies and pharmacological attributes, as established by linear regression models, are shown in Table 6. Since (R) is greater than the critical value of 0.5 and the p-value is less than 0.05, the highest value of (R) indicates that all features are statistically significant. For these computations, Pearson's correlation coefficient was employed (Arockiaraj *et al.* 2024). The linear, quadratic, cubic and logarithmic regression models for different entropies values are compared in Fig. 3 to 5. The regression equations in section 3 offer the most precise approximation for the physicochemical properties of the medications in question. For (MR) and (P), the most accurate predictor is the A1, A2, A3, A4, A5 and A6. For (MV) and (P), on the other hand, the A7, A8, A9, A10, A11 and A12 entropies are the most reliable predictor.

The effective models that predicted properties efficiently and are discussed below:

$$MR = 19.141 + 342.217 * (A9) + -316.248 (A9)^2$$

$$BP = 916.301 + 0 (A2) + -534.462 (A2)^2 + 196.605 (A2)^3$$

$$MW = 710.188 + 0(A3) + -846.515(A3)^2 + 404.8940 (A3)^3$$

$$Comp = 13166.867 + -13759.027 (A9) + 3687.109 (A9)^2 + 0.0001 (A9)^3$$

$$MV = 587.930 + 0 (A11) + 546.991 (A11)^2 + -165.285 (A11)^3$$

Table 14 demonstrates that novel entropy indices are the most accurate predictors for each attribute. It is clear from Table 3 to Table 14 that the features BP and E are best predicted by the degree-based indices in QRM, whilst the remaining qualities are well predicted by the cubic entropies. The most accurate predictor of the attributes according to our QSPR research using linear, quadratic, cubic and logarithmic the best predictors for the qualities FP and logP are BP, E, the entropies with A1, A2, A3, A4, A5, A6, A7, A8, A9, A10, A11 and A12, respectively, while the greatest predictor for the qualities MV and MR is the index RI. In addition to the key predictors, the statistical measurements including R2, RMSE, p-value, and F-Stat. Fig. 3 to 5 provide a graphical illustration of regression models. In order to forecast the physical characteristics, the study focusses on psoriasis medications using degree-based entropies. This problem can cause the analysis to call for more

processing power. However, to overcome these scaling issues, optimization methods and more effective algorithms might be created.

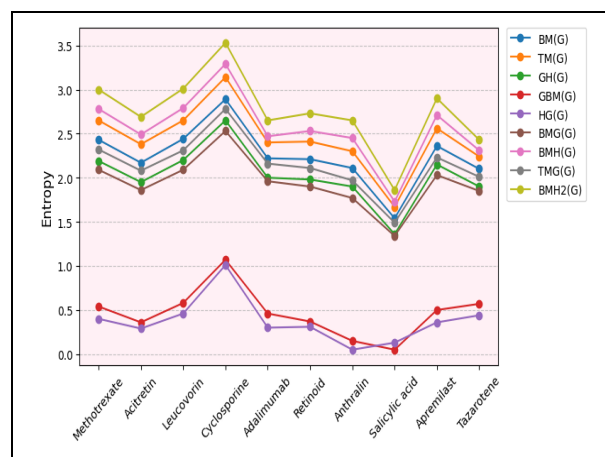
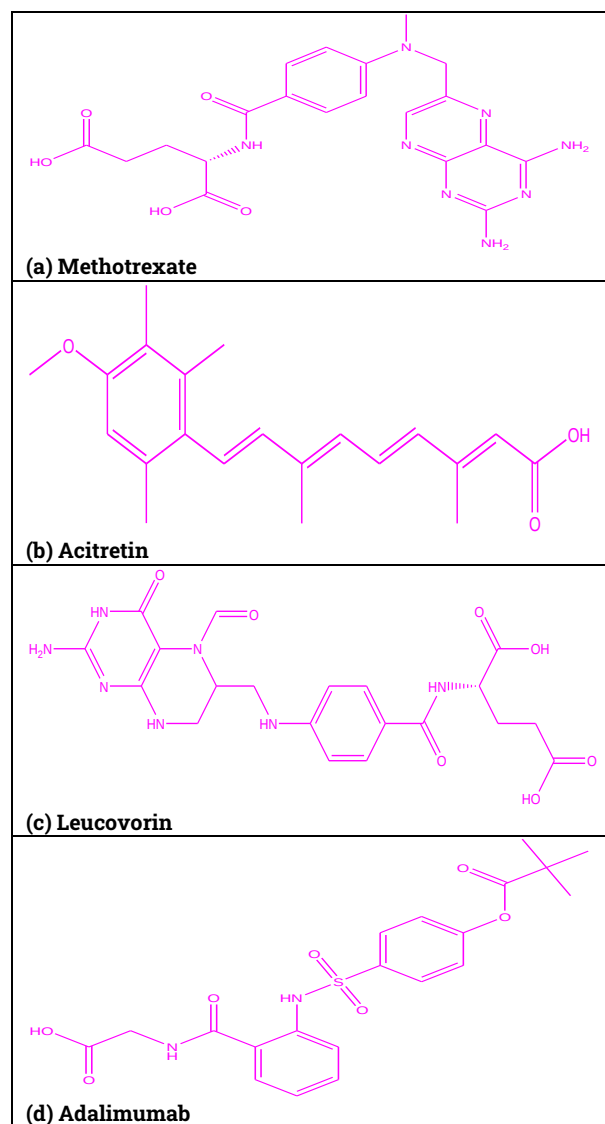


Fig. 1: Comparison of entropy values of psoriasis drugs



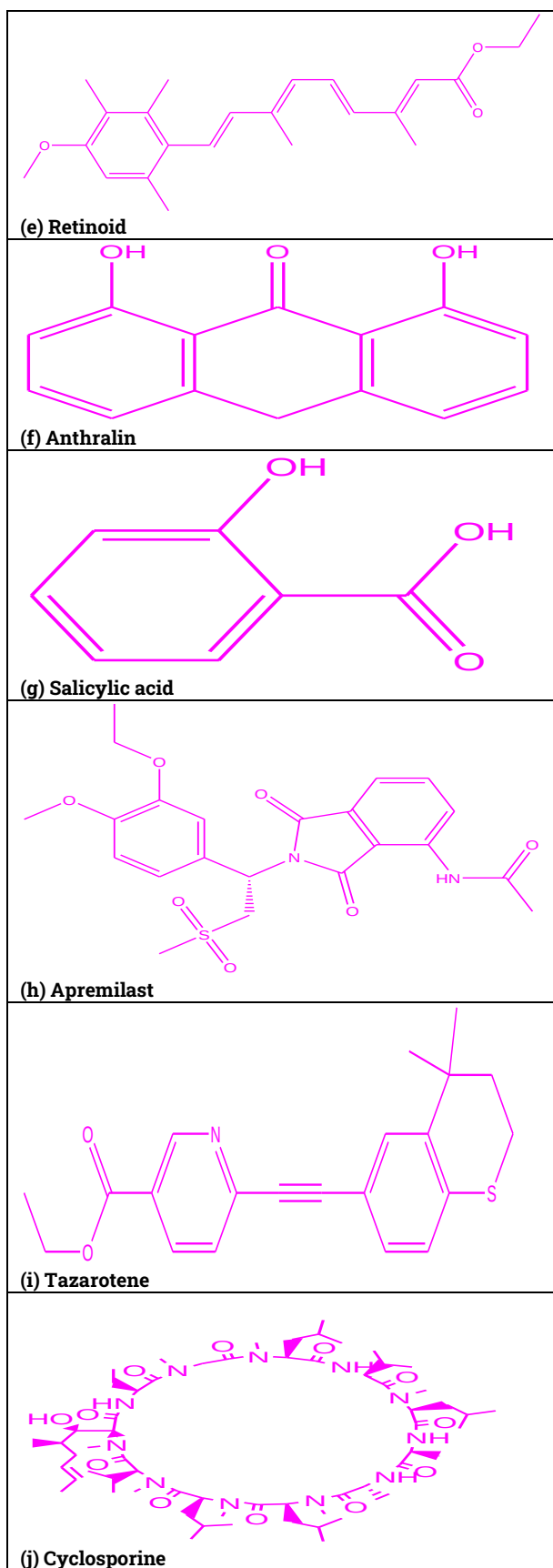


Fig. 2: Psoriasis treatment drugs

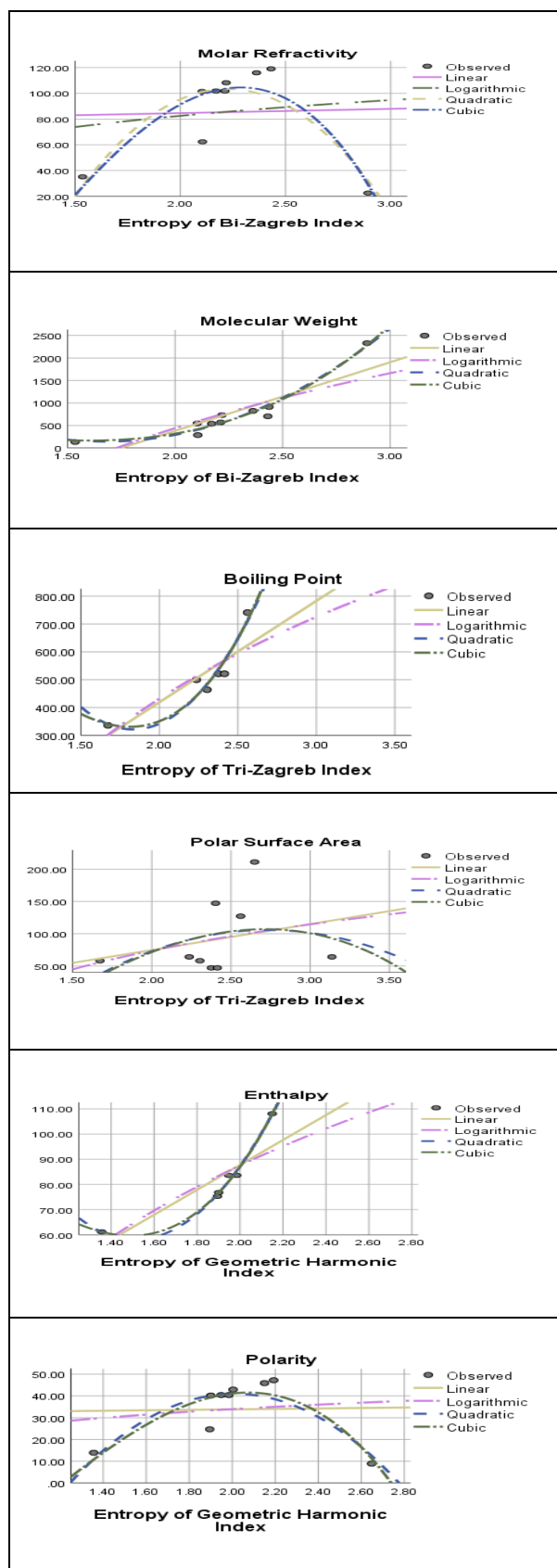


Fig. 3: Regression models of HM (G) with complexity, flash point, refractive index

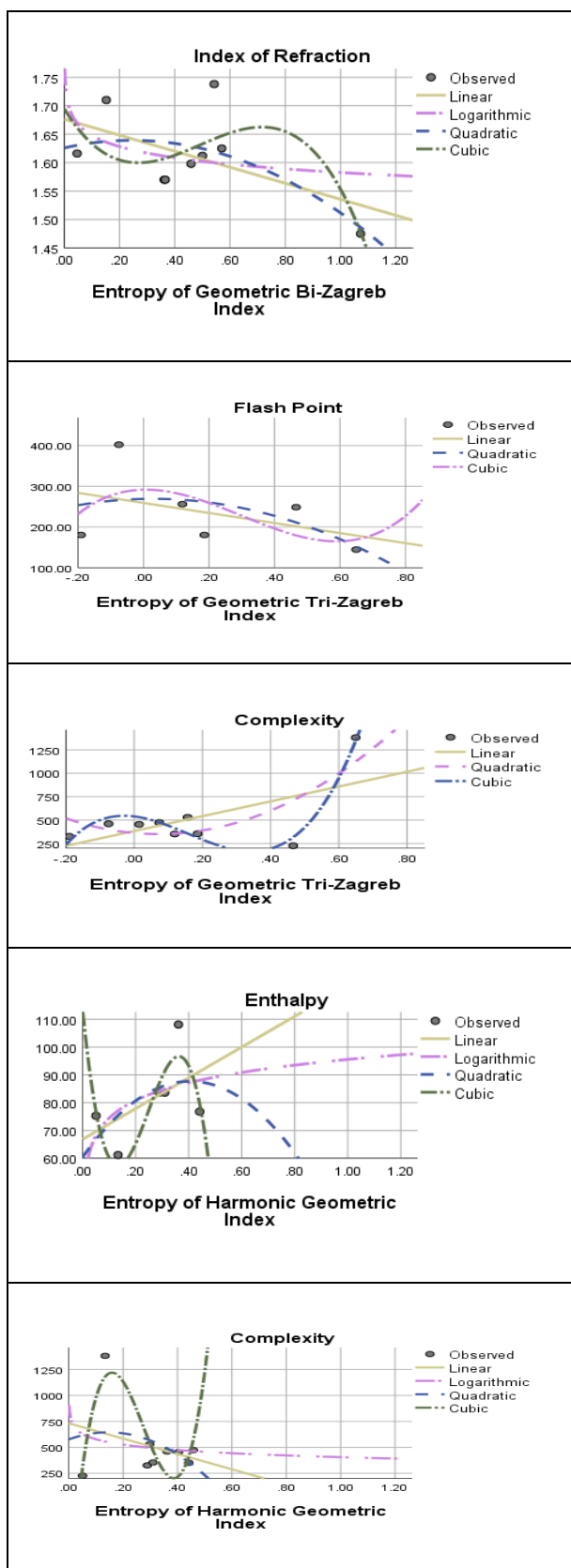


Fig. 4: Logarithmic regression model of HM (G) with complexity, flash point, refractive Index

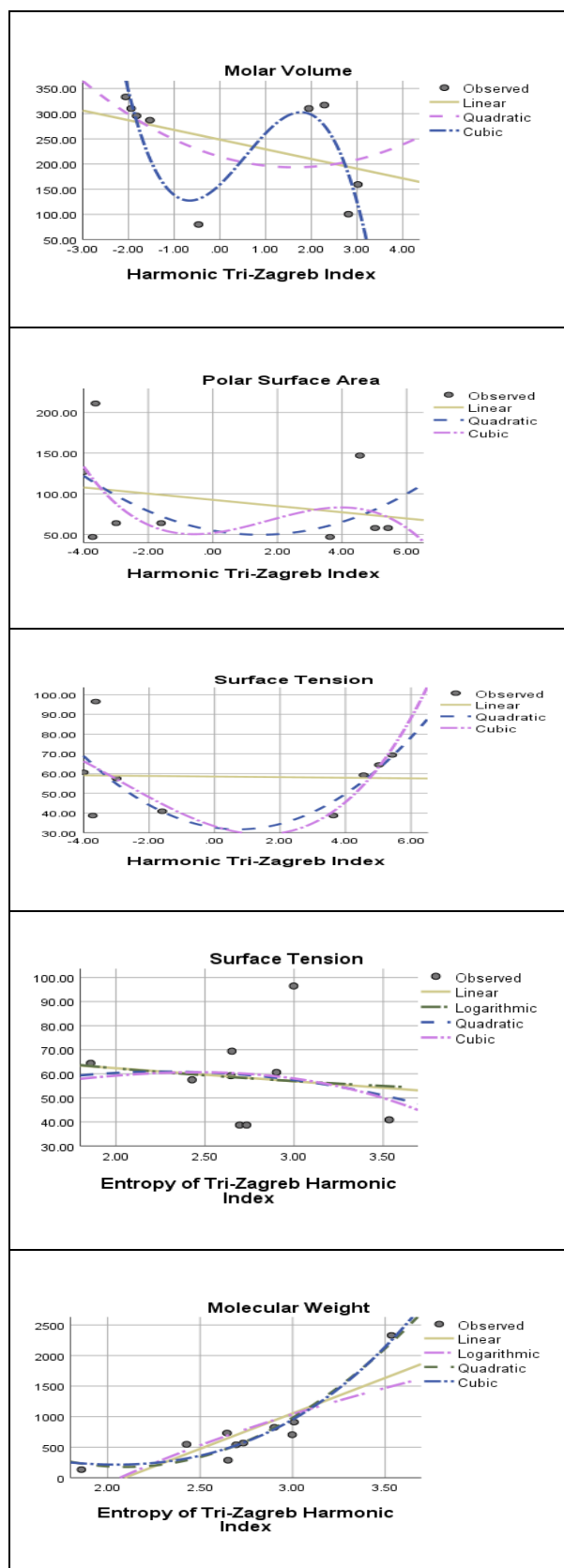


Fig. 5: Logarithmic regression model of HM (G) with complexity, flash point, refractive Index

Table 1. Formulae to compute the entropy on the base of

Descriptor	Topological Indices	Entropy (ENT _{Ti})
Bi-Zagreb (A ₁)	$BM(r, x) = r + x + rx$	$ENT_{BM} = \log(BM) - \frac{1}{BM} \log(\prod (r + x + rx)^{(r+x+rx)})$
Tri-Zagreb(A ₂)	$TM(r, x) = r^2 + x^2 + rx$	$ENT_{TM} = \log(BM) - \frac{1}{BM} \log(\prod (r^2 + x^2 + rx)^{(r^2+x^2+rx)})$
Geometric3 Harmonic(A ₃)	$GH(r, x) = \frac{(r+x)\sqrt{rx}}{2}$	$ENT_{GH} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{(r+x)\sqrt{rx}}{2})^{(\frac{(r+x)\sqrt{rx}}{2})})$
Geometric Bi-Zagreb(A ₄)	$GBM(r, x) = \frac{\sqrt{rx}}{r+x+rx}$	$ENT_{GBM} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{\sqrt{rx}}{r+x+rx})^{(\frac{\sqrt{rx}}{r+x+rx})})$
Geometric Tri-Zagreb(A ₅)	$GTM(r, x) = \frac{\sqrt{rx}}{r^2+x^2+rx}$	$ENT_{GTM} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{\sqrt{rx}}{r^2+x^2+rx})^{(\frac{\sqrt{rx}}{r^2+x^2+rx})})$
Harmonic Geometric(A ₆)	$HG(r, x) = \frac{2}{(r+x)\sqrt{rx}}$	$ENT_{HG} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{2}{(r+x)\sqrt{rx}})^{(\frac{2}{(r+x)\sqrt{rx}})})$
Harmonic- Bi-Zagreb(A ₇)	$HBM(r, x) = \frac{2}{(r+x+rx)(r+x)}$	$ENT_{HBM} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{2}{(r+x+rx)(r+x)})^{(\frac{2}{(r+x+rx)(r+x)})})$
Harmonic- Tri-Zagreb(A ₈)	$HTM(r, x) = \frac{2}{(r^2+x^2+rx)(r+x)}$	$ENT_{HTM} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{2}{(r^2+x^2+rx)(r+x)})^{(\frac{2}{(r^2+x^2+rx)(r+x)})})$
Bi-Zagreb Geometric(A ₉)	$BMG(r, x) = \frac{r+x+rx}{\sqrt{rx}}$	$ENT_{BMG} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{r+x+rx}{\sqrt{rx}})^{(\frac{r+x+rx}{\sqrt{rx}})})$
Bi-Zagreb Harmonic(A ₁₀)	$BMH(r, x) = \frac{(r+x+rx)(r+x)}{2}$	$ENT_{BMH} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{(r+x+rx)(r+x)}{2})^{(\frac{(r+x+rx)(r+x)}{2})})$
Tri-Zagreb Geometric(A ₁₁)	$TMG(r, x) = \frac{r^2+x^2+rx}{\sqrt{rx}}$	$ENT_{TMG} = \log(BM) - \frac{1}{BM} \log(\prod (\frac{r^2+x^2+rx}{\sqrt{rx}})^{(\frac{r^2+x^2+rx}{\sqrt{rx}})})$
Tri-Zagreb Harmonic(A ₁₂)	$BMH(r, x) = \frac{(r^2+x^2+rx)(r+x)}{2}$	$ENT_{BMH} = \log(BM) - \frac{1}{BM} \log[\prod (\frac{(r^2+x^2+rx)(r+x)}{2})^{(\frac{(r^2+x^2+rx)(r+x)}{2})}]$

Table 2. Entropy of psoriasis drugs

Drugs	BM	TM	GH	GBM	GTM	HTM	BMG	BMH	TMG	BMH
Methotrexate	2.43	2.65	2.19	0.54	0.01	-3.63	2.09	2.78	2.32	3.00
Acitretin	2.17	2.38	1.95	0.36	-0.19	-3.72	1.86	2.49	2.08	2.69
Leucovorin	2.44	2.65	2.20	0.58	0.07	-3.27	2.09	2.79	2.31	3.01
Cyclosporine	2.89	3.14	2.65	1.07	0.64	-1.60	2.53	3.29	2.78	3.53
Adalimumab	2.22	2.40	2.00	0.46	0.16	4.55	1.96	2.47	2.16	2.65
Retinoid	2.21	2.41	1.98	0.37	0.19	3.63	1.90	2.53	2.11	2.73
Anthralin	2.11	2.30	1.9	0.15	0.47	5.43	1.77	2.45	1.97	2.65
Salicylic acid	1.54	1.67	1.36	0.05	0.65	5.02	1.34	1.73	1.49	1.86
Apremilast	2.36	2.56	2.15	0.50	-0.08	-4.00	2.03	2.71	2.23	2.90
Tazarotene	2.10	2.24	1.9	0.57	0.12	-2.99	1.85	2.31	2.01	2.43

Table 3. Regression model for A3

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.766	0.749	0.452	0.13	0.001	0.071	0.001	0.021	0.001	0.577	0.765
f	13.092	11.937	3.301	1.05	0.005	0.539	0.004	0.153	0.009	9.543	26.062
p	0.022	0.026	0.143	0.34	0.948	0.487	0.949	0.708	0.927	0.018	0.001
A	- 282.675	-11.246	- 196.348	1.779	79.898	0.484	31.699	74.346	222.145	2486.81	- 2517.34
b	425.498	49.501	230.558	-0.083	2.706	45.284	1.063	-7.922	10.753	- 1010.81	1614.70 9
Quadratic Regression Model											
r	0.983	0.993	0.693	0.335	0.771	0.138	0.772	0.037	0.745	0.943	0.962
f	86.557	201.441	3.381	1.512	10.104	0.479	10.131	0.117	8.769	49.653	89.7
p	0.002	0.001	0.17	0.294	0.012	0.641	0.012	0.892	0.017	0	0
A	2529.31 5	339.262	1891.57 9	1.013	- 610.066	- 321.709	- 242.105	23.601	- 1674.88	11070.6 4	3585.46
b	- 2952.34	- 371.538	- 2277.51	0.702	709.679	375.42	281.617	44.074	1954.54 4	- 10924.3	- 4647.84
c	984.932	122.769	731.32	-0.196	- 176.495	-82.418	-70.04	-12.981	- 485.265	2781.43 6	1567.88 9
Cubic Regression Model											
r	0.984	0.993	0.703	0.356	0.817	0.152	0.817	0.049	0.779	0.943	0.967
f	94.295	203.378	3.553	1.659	13.375	0.539	13.409	0.153	10.581	49.653	103.316
p	0.002	0.001	0.162	0.267	0.006	0.609	0.006	0.861	0.011	0	0

A	820.357	123.818	586.099	1.435	-175.074	-245.333	-69.483	44.461	-471.952	11070.64	710.188
b	0	0	0	0	0	233.431	0	0	0	-10924.3	0
c	-680.351	-86.396	-566.952	0.178	195.048	0	77.391	14.591	534.427	2781.436	-846.516
d	307.913	38.596	242.724	-0.064	-62.683	-15.154	-24.872	-5.321	-171.498	0	404.894

Logarithmic Regression Model											
r	0.714	0.695	0.412	0.09	0.019	0.085	0.019	0.018	0.022	0.648	0.655
f	10.008	9.12	2.804	0.694	0.139	0.654	0.138	0.126	0.158	12.864	15.21
p	0.034	0.039	0.169	0.432	0.721	0.445	0.721	0.733	0.703	0.009	0.005
A	86.626	31.843	6.423	1.703	65.858	26.408	26.119	67.911	185.618	1745.697	-1231.89
b	692.379	80.347	370.855	-0.132	28.468	95.065	11.277	-13.854	84.964	-1867.27	2863.614

Table 4. Regression model for A1

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.748	0.735	0.421	0.126	0.001	0.073	0.001	0.021	0.002	0.577	0.755
F	11.849	11.087	2.91	1.011	0.007	0.553	0.007	0.148	0.013	9.54	24.659
p	0.026	0.029	0.163	0.348	0.933	0.481	0.934	0.712	0.913	0.018	0.001
A	-316.993	-15.489	-204.529	1.785	77.971	-5.625	30.932	74.943	216.857	2577.015	-2666.19
b	399.271	46.571	211.343	-0.077	3.309	43.621	1.304	-7.419	12.083	-952.142	1524.059
A1	Quadratic Regression Model										
r	0.967	0.987	0.63	0.326	0.766	0.134	0.767	0.034	0.744	0.941	0.957
F	43.356	112.214	2.558	1.451	9.83	0.465	9.855	0.107	8.713	47.464	77.319
p	0.006	0.002	0.225	0.306	0.013	0.649	0.013	0.9	0.017	0	0
A	3017.571	405.331	2094.469	0.944	-686.053	-348.647	-272.261	22.683	-1888.6	12020.1	4197.813
b	-3186.2	-405.913	-2260.64	0.7	710.037	360.919	281.759	40.922	1959.65	-10699.4	-4834.43

c	938.384	118.423	646.964	-0.176	$-\frac{159.667}{7}$	-71.685	-63.362	-10.921	$-\frac{440.002}{4}$	$\frac{2451.32}{4}$	$\frac{1440.22}{7}$
A1	Cubic Regression Model										
r	0.969	0.988	0.642	0.346	0.81	0.147	0.811	0.044	0.777	0.941	0.962
F	47.314	124.496	2.691	1.587	12.804	0.518	12.836	0.138	10.449	47.464	88.959
p	0.005	0.001	0.214	0.28	0.007	0.62	0.007	0.873	0.011	0	0
A	963.638	143.121	653.582	1.414	$-\frac{200.704}{7}$	$-\frac{265.727}{7}$	-79.656	44.35	$-\frac{543.998}{7}$	12020.1	868.839
b	0	0	0	0	0	223.421	0	0	0	-10699.4	0
c	-680.165	-87.311	-515.414	0.16	175.055	0	69.46	12.151	480.762	$\frac{2451.32}{4}$	-824.705
d	270.122	34.254	196.456	-0.052	-51.028	-11.896	-20.248	-4.032	$-\frac{139.954}{7}$	0	343.674
A1	Logarithmic Regression Model										
r	0.702	0.686	0.389	0.089	0.02	0.086	0.02	0.018	0.022	0.644	0.652
f	9.41	8.744	2.544	0.685	0.14	0.66	0.14	0.125	0.159	12.679	14.977
p	0.037	0.042	0.186	0.435	0.719	0.443	0.72	0.734	0.702	0.009	0.005
A	-13.049	20.125	-41.315	1.722	61.539	12.052	24.405	69.904	172.946	$\frac{2014.51}{4}$	-1647.1
b	727.843	84.671	382.047	-0.139	30.199	100.764	11.966	-14.558	89.856	-1961.49	$\frac{3012.62}{9}$

Table 5. Regression model for A2

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.732	0.732	0.388	0.122	0.001	0.073	0.001	0.02	0.001	0.568	0.743
f	10.9	10.921	2.537	0.972	0.005	0.552	0.005	0.146	0.009	9.201	23.113
p	0.03	0.03	0.186	0.357	0.945	0.482	0.945	0.713	0.925	0.019	0.001
A	-307.624	-15.248	-186.707	1.782	79.219	-5.491	31.423	74.865	220.616	$\frac{2549.17}{5}$	-2636.42
b	363.453	42.77	186.693	-0.07	2.53	40.106	0.997	-6.798	9.569	-864.436	$\frac{1390.62}{8}$
Quadratic Regression Model											
r	0.914	0.956	0.536	0.32	0.759	0.133	0.76	0.033	0.739	0.939	0.946
f	15.893	32.666	1.732	1.412	9.474	0.459	9.498	0.103	8.487	46.006	60.852
p	0.025	0.009	0.316	0.314	0.014	0.652	0.014	0.903	0.018	0	0

A	2774.18 ₂	386.909	1770.93 ₁	0.933	-692.673	-350.002	-274.893	23.707	-1908.83	12063.9	4348.47 ₂
b	-2677.5	-354.056	-1744.99	0.653	659.824	333.47	261.837	36.764	1822.86 ₉	-9867.25	-4565.98
c	730.807	95.366	464.226	-0.15	-136.706	-61.015	-54.25	-9.06	-377.136	2076.69 ₇	1242.00 ₅
Cubic Regression Model											
r	0.92	0.961	0.55	0.341	0.8	0.145	0.8	0.043	0.769	0.939	0.953
f	17.304	36.844	1.837	1.551	12.002	0.51	12.033	0.133	9.968	46.006	70.558
p	0.023	0.008	0.301	0.287	0.008	0.624	0.008	0.878	0.012	0	0
A	916.301	140.183	580.065	1.409	-201.275	-266.05	-79.887	44.761	-546.131	12063.9	939.679
b	0	0	0	0	0	205.967	0	0	0	-9867.25	0
c	-534.463	-71.189	-374.743	0.138	149.071	0	59.151	10.084	409.756	2076.69 ₇	-731.868
d	196.606	25.76	132.657	-0.041	-40.057	-9.305	-15.895	-3.089	-109.969	0	276.468
Logarithmic Regression Model											
r	0.69	0.686	0.362	0.086	0.018	0.086	0.018	0.018	0.02	0.636	0.643
f	8.916	8.744	2.272	0.661	0.126	0.656	0.125	0.125	0.143	12.236	14.379
p	0.041	0.042	0.206	0.443	0.733	0.445	0.734	0.734	0.717	0.01	0.005
A	-69.828	12.96	-62.916	1.732	60.373	3.879	23.941	71.114	169.389	2162.81 ₇	-1878.29
b	723.632	84.875	369.669	-0.137	28.672	100.587	11.363	-14.566	85.413	-1944.37	2991.61 ₉

Table 6. Regression model for A4

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.523	0.453	0.328	0.28	0.009	0.032	0.009	0.051	0.004	0.278	0.87
f	4.384	3.312	1.955	2.724	0.065	0.235	0.065	0.375	0.03	2.702	53.473
p	0.104	0.143	0.235	0.143	0.806	0.643	0.806	0.56	0.867	0.144	0
A	356.658	64.209	147.41	1.676	90.692	75.41	35.967	64.855	254.003	886.344	-179.568
b	472.778	51.767	264.198	-0.141	-11.846	35.449	-4.717	-14.197	-22.679	-956.866	2016.67 ₉
Quadratic Regression Model											
r	0.597	0.571	0.344	0.385	0.983	0.254	0.983	0.078	0.96	0.606	0.957
f	2.225	2	0.785	1.878	168.947	1.021	169.551	0.253	72.744	4.611	78.649
p	0.256	0.281	0.532	0.233	0	0.415	0	0.784	0	0.061	0

A	285.894	53.708	170.084	1.626	19.141	21.068	7.582	58.784	55.572	1362.95 ₉	191.226
b	1208.05 ₂	160.877	28.602	0.109	342.218	304.357	135.744	15.844	959.245	-5571.48	222.277
c	-1205.82	-178.935	386.367	-0.223	-316.248	-240.187	-125.46	-26.833	-877.049	7170.04 ₆	1622.89 ₆
Cubic Regression Model											
r	0.632	0.629	0.346	0.485	0.983	0.404	0.983	0.407	0.972	0.968	0.971
f	1.143	1.132	0.353	1.568	94.169	1.131	94.589	1.143	56.848	49.894	67.056
p	0.498	0.501	0.796	0.307	0	0.421	0	0.417	0	0	0
A	369.458	66.499	154.378	1.695	18.379	83.764	7.242	88.474	25.583	2212.97 ₆	-13.576
b	-390.538	-83.812	329.05	-0.81	352.358	-529.794	140.271	-379.168	1358.23 ₁	-21339.1	2866.24 ₁
c	4983.88 ₁	768.493	-776.961	2.076	-341.605	1845.63 ₃	-136.78	960.906	-1874.73	65932.6	-4835.26
d	-6494.32	-994.055	1220.58	-1.407	15.518	-1276.51	6.928	-604.489	610.57	-59813.3	3912.07 ₁
Logarithmic Regression Model											
r	0.581	0.531	0.293	0.111	0.12	0.093	0.12	0.035	0.142	0.537	0.507
f	5.555	4.524	1.658	0.872	0.957	0.722	0.956	0.255	1.155	8.105	8.218
p	0.078	0.101	0.267	0.381	0.361	0.424	0.361	0.629	0.318	0.025	0.021
A	658.139	97.639	307.504	1.583	99.867	111.844	39.596	54.433	287.887	169.003	1250.73 ₉
b	105.109	11.814	52.628	-0.028	13.697	19.226	5.431	-3.77	41.602	-298.513	488.269

Table 7. Regression model for A5

Properti es	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.569	0.571	0.181	0.044	0.838	0.13	0.839	0.002	0.862	0.365	0.055
f	5.271	5.33	0.883	0.326	36.326	1.046	36.362	0.011	43.648	4.031	0.468
p	0.083	0.082	0.401	0.586	0.001	0.34	0.001	0.918	0	0.085	0.513
A	573.61 ₅	88.468	259.04 ₃	1.624	109.10 ₂	106.34 ₅	43.264	58.965	311.17 ₆	383.45 ₉	658.11 ₄
b	-310.10 ₉	-36.572	-123.35 ₅	-0.054	-108.71 ₁	-68.149	-43.131	-2.433	-308.40 ₈	791.12 ₂	486.91 ₂
Quadratic Regression Model											

r	0.617	0.6	0.245	0.181	0.973	0.19	0.973	0.07	0.964	0.581	0.089
f	2.412	2.251	0.486	0.662	109.08 ₂	0.703	109.89 ₄	0.226	79.745	4.162	0.342
p	0.237	0.253	0.656	0.55	0	0.532	0	0.804	0	0.073	0.722
A	585.65 ₅	89.564	268.83	1.63	111.69 ₂	109.09 ₁	44.291	59.906	317.47 ₈	361.90 ₇	645.96 ₃
b	- 137.39	- 20.851	17.039	0.157	- 11.334	35.135	-4.492	32.929	- 71.437	- 322.95 ₆	- 367.19 ₅
c	- 372.10 ₄	- 33.869	- 302.46 ₃	-0.398	- 184.07 ₇	- 195.24 ₄	- 73.042	- 66.847	- 447.95 ₉	2305.3 ₀₄	1589.8 ₈₇
Cubic Regression Model											
r	0.644	0.62	0.293	0.196	0.981	0.444	0.981	0.141	0.968	0.938	0.194
f	1.208	1.088	0.276	0.406	87.907	1.329	88.094	0.274	49.891	25.14	0.48
p	0.483	0.512	0.842	0.755	0	0.363	0	0.842	0	0.002	0.708
A	610.10 ₇	92.007	291.51 ₄	1.62	114.97 ₅	138.23 ₆	45.581	64.836	323.85 ₃	539.09 ₈	825.57 ₂
b	- 138.03 ₅	- 20.915	16.44	0.159	- 12.017	29.074	-4.76	31.904	- 72.763	- 448.93 ₅	- 461.85 ₈
c	- 1287.4 ₄	- 125.34	- 1151.6 ₁	0.052	- 337.39	- 1556.3 ₃	- 133.28 ₇	- 297.11 ₉	- 745.68 ₂	- 6851.6 ₅	- 7672.7 ₅
d	1388.0 ₈₈	138.71 ₄	1287.7 ₁₇	-0.687	233.68 ₂	2074.5 ₉₁	91.827	350.98 ₅	453.79 ₅	14567.27	14343.22

Table 8. Regression model for A6

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.319	0.273	0.138	0.409	0.085	0.002	0.085	0.093	0.061	0.088	0.915
f	1.871	1.504	0.642	4.836	0.648	0.012	0.649	0.721	0.458	0.675	85.963
p	0.243	0.287	0.468	0.064	0.447	0.915	0.447	0.424	0.52	0.438	0
A	379.76 ₈	66.813	172.95 ₁	1.68	99.548	88.197	39.478	66.034	277.60 ₁	732.01 ₄	- 83.088
b	507.674	55.31	235.93	-0.184	-38.849	8.874	-15.427	-20.772	-92.529	- 739.426	2240.52 ₁
Quadratic Regression Model											
r	0.325	0.303	0.243	0.424	0.833	0.211	0.833	0.105	0.824	0.114	0.947
f	0.723	0.653	0.48	2.208	14.989	0.804	14.989	0.351	14.066	0.385	62.232

p	0.554	0.581	0.659	0.191	0.005	0.491	0.005	0.718	0.005	0.696	0
A	354.18 ₂	60.384	244.67 ₁	1.657	26.448	26.627	10.481	61.446	71.099	576.51 ₅	174.13 ₈
b	823.179	134.583	-648.459	-0.062	354.159	339.891	140.469	3.896	1017.67 ₇	947.631	901.487
c	-660.155	-165.868	1850.47 ₃	-0.11	-355.804	-299.682	-141.138	-22.333	-1005.11	-3274.37	1226.51 ₃
Cubic Regression Model											
r	0.804	0.81	0.545	0.759	0.842	0.236	0.842	0.377	0.826	0.724	0.949
f	2.729	2.838	0.8	5.246	8.888	0.516	8.882	1.007	7.9	4.369	36.905
p	0.28	0.271	0.597	0.053	0.019	0.689	0.019	0.462	0.024	0.073	0
A	793.76 ₅	113.58 ₉	491.29 ₅	1.81	38.014	57.544	15.048	94.099	57.495	-975.35 ₆	85.974
b	-8190.67	-956.405	-5705.59	-2.283	186.363	-108.624	74.208	-469.813	1215.03 ₉	32007.2 ₂	2113.42 ₁
c	41058.1 ₄	4883.49	25256.1 ₃	6.512	144.548	1037.74 ₆	56.448	1390.22	-1593.62	-142091	-2246.86
d	-54110.2	-6549.21	-30358	-4.548	-343.658	-918.589	-135.708	-970.187	404.211	173778	2348.71 ₇
Logarithmic Regression Model											
r	0.254	0.235	0.056	0.338	0.013	0.049	0.013	0.078	0.03	0.025	0.56
f	1.361	1.226	0.238	3.581	0.091	0.363	0.091	0.591	0.214	0.177	10.18
p	0.308	0.33	0.651	0.1	0.771	0.566	0.772	0.467	0.658	0.687	0.013
A	638.813	95.551	276.724	1.544	91.547	110.791	36.293	50.649	270.144	405.355	1440.74 ₁
b	81.047	9.165	26.881	-0.054	4.925	15.334	1.95	-6.169	20.923	-74.901	563.029

Table 9. Regression model for A7

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.461	0.421	0.27	0.004	0.189	0.089	0.189	0.002	0.179	0.123	0.109
f	3.426	2.913	1.477	0.029	1.63	0.688	1.626	0.011	1.531	0.983	0.982
p	0.138	0.163	0.291	0.871	0.242	0.434	0.243	0.921	0.256	0.354	0.351
A	527.442	82.948	242.582	1.612	87.083	93.361	34.527	58.513	248.516	500.339	762.789
b	-36.162	-4.066	-19.497	0.002	-7.063	-7.738	-2.799	-0.323	-19.264	52.029	-91.254
Quadratic Regression Model											
r	0.464	0.425	0.374	0.497	0.249	0.108	0.248	0.247	0.204	0.151	0.633
f	1.301	1.109	0.896	2.96	0.992	0.362	0.989	0.986	0.768	0.533	6.038
p	0.392	0.436	0.495	0.128	0.424	0.71	0.425	0.426	0.505	0.612	0.03

A	506.016	80.179	155.004	1.495	68.082	76.6	27.002	38.864	214.601	316.307	1754.592
b	-39.891	-4.548	-34.74	-0.021	-10.855	-11.083	-4.301	-4.245	-26.033	20.23	108.318
c	4.396	0.568	17.969	0.028	4.497	3.967	1.781	4.65	8.027	39.84	-235.373
Cubic Regression Model											
r	0.65	0.692	0.391	0.502	0.692	0.171	0.692	0.278	0.757	0.152	0.707
f	1.239	1.496	0.427	1.683	3.747	0.344	3.74	0.642	5.201	0.3	4.821
p	0.476	0.425	0.756	0.285	0.095	0.796	0.095	0.62	0.054	0.825	0.049
A	362.281	59.922	124.657	1.499	50.376	65.951	19.976	41.241	159.252	276.965	1869.182
b	48.784	7.949	-16.018	-0.03	24.879	10.41	9.878	-9.044	85.672	42.108	-141.488
c	51.146	7.157	27.839	0.025	14.899	10.223	5.908	3.254	40.544	52.87	-308.836
d	-21.217	-2.99	-4.479	0.002	-7.787	-4.684	-3.09	1.046	-24.343	-5.724	55.214

Table 10. Regression model for A8

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.457	0.417	0.274	0.007	0.147	0.079	0.147	0.001	0.138	0.116	0.133
f	3.371	2.857	1.511	0.047	1.209	0.597	1.206	0.008	1.119	0.921	1.228
p	0.14	0.166	0.286	0.835	0.308	0.465	0.308	0.93	0.325	0.369	0.3
A	524.83	82.653	241.249	1.612	86.312	92.582	34.221	58.478	246.394	503.368	754.417
b	-19.369	-2.175	-10.576	0.001	-3.28	-3.814	-1.3	-0.15	-8.879	26.75	-52.996
Quadratic Regression Model											
r	0.465	0.426	0.396	0.51	0.239	0.142	0.238	0.291	0.182	0.136	0.594
f	1.303	1.112	0.983	3.122	0.943	0.495	0.939	1.233	0.669	0.472	5.122
p	0.391	0.435	0.469	0.118	0.441	0.633	0.442	0.356	0.546	0.645	0.043
A	488.179	77.949	138.024	1.468	57.728	54.896	22.9	32.595	190.655	319.395	1882.58 ₈
b	-22.081	-2.523	-18.216	-0.011	-5.765	-7.089	-2.284	-2.399	-13.724	13.123	45.97
c	2.148	0.276	6.051	0.009	1.845	2.432	0.731	1.67	3.597	11.043	-72.998
Cubic Regression Model											
r	0.669	0.711	0.419	0.514	0.663	0.193	0.663	0.319	0.704	0.139	0.665
f	1.346	1.637	0.481	1.765	3.279	0.398	3.273	0.78	3.965	0.268	3.969
p	0.453	0.401	0.729	0.27	0.117	0.761	0.117	0.554	0.086	0.846	0.071
A	354.544	59.365	106.124	1.469	52.287	51.89	20.742	33.301	173.768	277.959	1912.44 ₇
b	31.663	4.951	-5.386	-0.016	15.756	4.802	6.256	-5.19	53.08	30.473	106.39 ₉
c	14.178	1.949	8.922	0.009	3.839	3.534	1.522	1.412	9.788	14.948	-87.158

d	-3.445	-0.479	-0.822	0	-1.255	-0.694	-0.498	0.163	-3.897	-1.156	8.974
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Table 11. Regression model for A9

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.756	0.732	0.42	0.159	0.001	0.075	0.001	0.027	0.002	0.54	0.797
f	12.416	10.942	2.897	1.319	0.004	0.568	0.004	0.192	0.012	8.216	31.4
p	0.024	0.03	0.164	0.289	0.95	0.476	0.95	0.675	0.917	0.024	0.001
A	342.108	-17.667	214.597	1.803	79.859	-5.209	31.682	76.872	218.466	2540.532	2712.68
b	477.745	55.304	251.081	-0.099	2.843	50.201	1.117	-9.577	13.13	1083.76	1786.812
Quadratic Regression Model											
r	0.963	0.959	0.618	0.351	0.809	0.156	0.81	0.043	0.785	0.938	0.976
f	38.875	34.748	2.429	1.624	12.748	0.553	12.781	0.136	10.954	45.623	144.864
p	0.007	0.008	0.236	0.273	0.007	0.602	0.007	0.876	0.01	0	0
A	3109.506	407.436	2170.073	0.984	699.512	396.924	277.585	19.993	1927.69	13166.87	3684.935
b	3804.61	472.113	2707.53	0.767	827.15	464.5	328.215	50.582	2283.021	-13759	4989.63
c	1295.727	159.583	895.199	-0.224	212.884	106.996	-84.476	-15.537	586.217	3687.109	1755.361
Cubic Regression Model											
r	0.967	0.963	0.633	0.366	0.857	0.172	0.857	0.053	0.823	0.938	0.979
f	44.381	38.878	2.582	1.73	17.997	0.622	18.045	0.169	13.931	45.623	162.884
p	0.006	0.007	0.223	0.255	0.003	0.568	0.003	0.849	0.006	0	0
A	1000.338	145.474	688.631	1.436	206.902	301.066	-82.109	44.11	563.717	13166.87	671.423
b	0	0	0	0	0	284.13	0	0	0	-13759	0
c	955.845	119.546	729.365	0.196	234.709	0	93.125	16.554	645.796	3687.109	-911.93
d	438.35	54.288	320.779	-0.074	-78.283	-20.221	-31.061	-6.344	214.952	0	461.771
Logarithmic Regression Model											
r	0.713	0.687	0.389	0.116	0.019	0.091	0.018	0.023	0.023	0.606	0.693
f	9.918	8.794	2.551	0.92	0.132	0.698	0.132	0.161	0.163	10.762	18.083
p	0.035	0.041	0.185	0.369	0.727	0.431	0.728	0.7	0.699	0.013	0.003
A	79.651	31.251	8.896	1.714	66.581	25.344	26.405	68.974	185.614	1711.18	1264.14

b	755.469	87.289	393.845	-0.157	29.169	102.818	11.555	-16.396	90.421	- 1937.33	3098.47 2
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Table 12. Regression model for A10

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.724	0.728	0.396	0.106	0.001	0.067	0.001	0.018	0.001	0.578	0.716
f	10.479	10.725	2.626	0.829	0.004	0.504	0.004	0.127	0.006	9.607	20.202
p	0.032	0.031	0.18	0.393	0.952	0.501	0.952	0.732	0.939	0.017	0.002
A	- 265.39 2	- 10.547	- 171.41 6	1.767	80.102	0.535	31.774	73.417	225.36 9	2492.3 85	- 2498.9 7
b	328.66 6	38.789	171.52 4	-0.061	2.068	35.932	0.814	-5.922	7.263	- 802.45 5	1273.8 87
Quadratic Regression Model											
r	0.886	0.931	0.552	0.307	0.743	0.121	0.743	0.03	0.723	0.941	0.928
f	11.662	20.139	1.85	1.328	8.669	0.412	8.692	0.092	7.814	47.934	44.899
p	0.038	0.018	0.3	0.333	0.017	0.68	0.017	0.913	0.021	0	0
A	2335.0 01	331.03 9	1625.9 81	0.946	- 652.99 7	- 312.98 1	- 259.15 8	25.799	- 1797.2 7	11192. 33	4358.5 81
b	- 2125.8 3	- 283.63 1	- 1525.0 3	0.61	601.68 8	292.36 4	238.77 4	33.026	1661.6 28	- 8681.0 1	- 4342.8 8
c	563.02 8	73.959	389.16 6	-0.134	- 119.62 9	-51.16	- 47.475	-7.77	- 330.05 8	1736.7 05	1123.2 03
Cubic Regression Model											
r	0.895	0.938	0.57	0.332	0.779	0.132	0.78	0.039	0.747	0.941	0.938
f	12.767	22.587	1.987	1.492	10.579	0.456	10.607	0.123	8.85	47.934	52.886
p	0.034	0.016	0.282	0.298	0.011	0.654	0.011	0.886	0.016	0	0
A	804.08 1	125.51 2	543.96 3	1.406	- 185.47 3	- 236.26 9	-73.62	44.972	- 500.49 1	11192. 33	1000.8 29
b	0	0	0	0	0	180.71 6	0	0	0	- 8681.0 1	0
c	- 403.62 3	-54.18	- 314.95	0.126	129.85 3	0	51.527	8.963	356.26 3	1736.7 05	- 685.97
d	144.36 8	19.012	106.76 6	-0.036	- 33.452	-7.467	- 13.275	-2.611	- 91.706	0	243.86
Logarithmic Regression Model											
r	0.683	0.682	0.368	0.073	0.017	0.079	0.017	0.015	0.018	0.649	0.616
f	8.605	8.587	2.328	0.55	0.12	0.598	0.119	0.108	0.13	12.945	12.837
p	0.043	0.043	0.202	0.483	0.74	0.465	0.74	0.752	0.729	0.009	0.007
A	- 70.243	12.726	- 67.149	1.724	60.394	5.519	23.95	70.523	171.14	2200.4 06	- 1880.2 9

b	684.34 3	80.484	354.30 8	-0.122	27.237	93.841	10.794	- 13.204	79.293	- 1887.5 6	2846.1 86
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Table 13. Regression model for A11											
Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.752	0.741	0.392	0.153	0.001	0.077	0	0.026	0.001	0.537	0.787
f	12.103	11.465	2.58	1.267	0.004	0.586	0.003	0.187	0.01	8.13	29.628
p	0.025	0.028	0.183	0.297	0.954	0.469	0.955	0.678	0.923	0.025	0.001
A	- 357.096	- 20.342	- 208.391	1.803	80.259	-8.383	31.837	76.967	219.737	2559.34	- 2749.79
b	439.913	51.4	224.086	-0.089	2.387	46.958	0.939	-8.718	11.293	- 989.691	1635.365
Quadratic Regression Model											
r	0.947	0.972	0.541	0.345	0.8	0.154	0.8	0.041	0.777	0.938	0.969
f	27.071	51.733	1.77	1.579	11.976	0.548	12.007	0.129	10.45	45.499	108.996
p	0.012	0.005	0.311	0.281	0.008	0.605	0.008	0.881	0.011	0	0
A	3150.8 35	427.29 6	1950.5 73	0.952	- 726.602	- 407.35	- 288.341	20.227	- 2004.38	13410. 33	3954.8 67
b	- 3486.52	- 449.642	- 2192.44	0.725	775.251	429.114	307.627	45.632	2141.6 98	- 12645.5	- 4796.53
c	1073.03	136.927	660.399	-0.191	- 180.909	- 89.454	- 71.788	- 12.722	- 498.677	3057.00 3	1510.00 4
Cubic Regression Model											
r	0.952	0.975	0.555	0.36	0.845	0.17	0.846	0.051	0.813	0.938	0.972
f	29.718	59.35	1.867	1.687	16.384	0.614	16.429	0.16	13.046	45.499	123.654
p	0.011	0.004	0.297	0.262	0.004	0.572	0.004	0.856	0.007	0	0
A	1012.91 2	150.965	629.699	1.425	- 215.464	- 309.566	-85.511	44.203	-587.93	13410.3 3	758.475
b	0	0	0	0	0	262.68	0	0	0	- 12645.5	0
c	- 793.915	- 103.278	- 535.415	0.168	198.628	0	78.812	13.566	546.991	3057.00 3	-816.56
d	329.076	42.236	214.76	-0.057	-60.138	-15.337	-23.862	-4.722	- 165.286	0	365.865
Logarithmic Regression Model											
r	0.71	0.696	0.367	0.113	0.017	0.092	0.017	0.022	0.021	0.603	0.687
f	9.782	9.173	2.318	0.89	0.122	0.713	0.121	0.159	0.15	10.649	17.558
p	0.035	0.039	0.203	0.377	0.737	0.426	0.738	0.702	0.71	0.014	0.003
A	-6.913	20.736	-28.791	1.73	64.134	12.972	25.434	70.742	177.942	1924.378	-1603.17

b	771.543	89.907	391.204	-0.158	28.554	105.698	11.314	-16.58	88.632	-1963.69	3138.988
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Table 14. Regression model for A12

Properties	BP	EP	FP	IR	MR	PSA	POL	ST	MV	COMP	MW
Linear Regression Model											
N	6	6	6	9	9	9	9	9	9	9	10
r	0.695	0.712	0.358	0.102	0	0.066	0	0.018	0	0.56	0.701
f	9.127	9.901	2.234	0.795	0.002	0.493	0.002	0.125	0.003	8.911	18.712
p	0.039	0.035	0.209	0.402	0.968	0.505	0.969	0.734	0.957	0.02	0.003
A	-239.561	-8.291	-146.195	1.763	81.953	2.34	32.504	73.175	230.83	2427.211	-2427.75
b	296.181	35.267	149.957	-0.055	1.245	32.811	0.489	-5.428	4.756	-722.866	1160.444
Quadratic Regression Model											
r	0.814	0.872	0.461	0.302	0.738	0.12	0.738	0.029	0.719	0.935	0.914
f	6.568	10.219	1.282	1.299	8.435	0.409	8.457	0.09	7.667	42.888	37.338
p	0.08	0.046	0.396	0.34	0.018	0.681	0.018	0.915	0.022	0	0
A	2023.622	300.47	1335.873	0.939	-652.052	-314.313	-258.787	26.246	-1796.33	11268.69	4502.109
b	-1686.24	-235.19	-1148.25	0.572	560.586	274.113	222.465	30.334	1549.534	-8151.52	-4127.73
c	422.157	57.594	276.454	-0.117	-103.918	-44.831	-41.24	-6.644	-286.999	1519.635	984.737
Cubic Regression Model											
r	0.827	0.884	0.481	0.328	0.768	0.131	0.769	0.039	0.738	0.935	0.927
f	7.181	11.456	1.391	1.466	9.947	0.451	9.974	0.12	8.437	42.888	44.377
p	0.072	0.039	0.374	0.303	0.012	0.657	0.012	0.889	0.018	0	0
A	750.316	120.785	488.125	1.403	-182.048	-235.228	-72.265	45.197	-491.484	11268.69	1080.348
b	0	0	0	0	0	168.202	0	0	0	-8151.52	0
c	-309.87	-43.323	-232.965	0.11	111.724	0	44.334	7.665	306.743	1519.635	-619.561
d	104.373	14.228	74.124	-0.029	-26.846	-6.058	-10.653	-2.08	-73.654	0	201.799
Logarithmic Regression Model											
r	0.662	0.672	0.337	0.07	0.014	0.077	0.014	0.015	0.016	0.631	0.603
f	7.823	8.213	2.035	0.528	0.102	0.587	0.102	0.108	0.111	11.956	12.176
p	0.049	0.046	0.227	0.491	0.759	0.469	0.759	0.753	0.749	0.011	0.008
A	-102.654	8.3	-75.151	1.73	60.744	0.521	24.086	71.299	172.085	2284.397	-2024.98
b	667.461	79.164	336.066	-0.119	24.933	92.196	9.883	-13.046	72.662	-1836.23	2788.927

5. CONCLUSION

The integration of computational molecular descriptors with nanotechnology offers a promising approach for understanding molecular structure, physicochemical behaviour and the design of nano-enabled therapeutic systems. In this study, degree-based topological indices and entropy descriptors were evaluated for ten commonly used drugs for psoriasis within a quantitative structure–property relationship (QSPR) framework. Molecular structures were represented as molecular graphs to systematically characterize structural connectivity,

branching and molecular complexity, and the resulting descriptors were correlated with selected physicochemical properties using linear, quadratic, cubic and logarithmic regression models. Several entropy-based descriptors exhibited meaningful relationships with the investigated properties, demonstrating their potential for describing structural variations among the selected pharmaceutical molecules. The developed computational framework provides an interpretable and resource-efficient approach for preliminary molecular screening and structure–property assessment, reducing reliance on extensive experimental investigation during early-stage analysis. From a nanotechnology perspective,

these descriptors can provide useful molecular-level information for the rational design and evaluation of nanostructured drug-delivery systems, where molecular size, connectivity, complexity and physicochemical characteristics can influence drug-carrier interactions, loading behaviour and release performance. Future studies should expand the molecular dataset, employ independent validation and incorporate machine-learning approaches to improve predictive robustness and generalization. Integration of entropy-based descriptors with molecular docking, molecular dynamics and nano-carrier simulations may further elucidate drug-target and drug-nanomaterial interactions. Such an integrated computational strategy could support the development of nano-enabled therapeutic platforms while providing a systematic basis for evaluating structure-property relationships across broader pharmaceutical and nanostructured molecular systems.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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