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Research Article

Computational Approaches to Predict NSAID Characteristics Using Degcity Indices and QSPR Analysis

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Abstract: Non-steroidal anti-inflammatory drugs (NSAIDs) represent a widely utilized class of medications renowned for their analgesic, antipyretic, and anti-inflam-matory properties. Commonly prescribed and available over the counter, these drugs play a critical role in managing a variety of conditions, including acute pain, chronic inflammatory diseases, and fever. This paper has concentrated on the application of degcity indices in Quantitative Structure-Property Relationship (QSPR) research of a few physicochemical aspects of non-steroidal anti-inflammatory drugs (NSAIDs). This study also sought to calculate the regression models and degcity indices for five non-steroidal anti-inflammatory drugs (NSAIDs). Additionally, the QSPR model provides a much more accurate estimate of the molecular weight, enthalpy, molar refraction, melting point, boiling point, and polarizability of pharmaceuticals. The drugs' molecular weight, enthalpy, molar refraction, melting and boiling points, and polarizability are all precisely predicted by the created QSPR model. For example, according to the $DC_1^*(G)$ index, the correlation coefficient for molar refraction and molecular weight are 0.9763 and 0.9731, respectively. Strong relationships were found between boiling point 0.9727 and complexity 0.9754 for several indices, including $DC_3^*(G)$ and $DC_5^*(G)$. Conversely, lesser associations were also observed, such as $DC_6^*(G)$ with polarizability 0.6307. These results highlight how useful degcity indices are for clarifying the physical properties of chemical compounds used in pharmaceutical research. The physical features of chemical compounds employed in the production of painkillers are strongly correlated with degcity indices, as demonstrated by the comparison of estimated and actual values for the medications.

***Keywords*:** degcity indices, nonsteroidal anti-inflamatory drug, QSPR analysis, physicochemical properties

MSC: 05C85, 05C92, 05C09, 62J05

1. Introduction

The area of mathematical chemistry that deals with chemical graph theory. Managing chemical graphs that depict chemical systems is an area of expertise. Thus, the examination of every effect of connection in a chemical system falls under the responsibility of chemical graph theory. It has been discovered to be a helpful tool in Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) [1–3]. Some studies in the aforementioned disciplines have been conducted using what are known as topological indices. Since topological indices can be computed with just the chemical compound's molecular structure and no extra experimental data, they are

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frequently utilized in QSPR research [4]. These days, topological indices play a unique role in QSPR analysis to forecast the physicochemical features of chemical compounds. For additional information on QSPR studies and applications, see [5–7]. Using topological indices, QSPR and QSAR are now essential tools for predicting the physicochemical properties of chemical molecules [8, 9]. In addition, predicting these characteristics reduces the time and expense associated with drug design. In their 2023 study, Rayer et al. and Johnson et al. [10–12] investigated the characteristics and uses of topological indices that are produced from zero-divisor networks connected to commutative rings. By applying graph theory, these indices provide insight into the rings' structure. With the use of computer methods, the study improved our knowledge of algebraic characteristics and has beneficial implications for network theory and chemistry [13]. The use of topological indices to forecast the biological and physical characteristics of anti-Alzheimer's medications, such as donepezil and tacrine, is covered in the study. Using linear regression, a quantitative structure-property relationship (QSPR) model is created to evaluate properties including molecular weight and boiling point [14]. In order to examine polycyclic aromatic hydrocarbons (PAHs) and determine the structural elements influencing their physicochemical characteristics, the study presents eccentricity topological descriptors. Regression analysis is used to show the predictive power of topological indices by correlating these attributes with medication attributes such as bioavailability, toxicity, and effectiveness [15]. The study highlights the need for novel treatments beyond the current cholinesterase inhibitors and N-methyl-D-aspartic acid (NMDA) antagonists in order to improve patient outcomes. It does this by discussing computational approaches, such as QSPR analysis and predictive mathematical modeling, to investigate novel therapeutic options for Alzheimer's disease.

Using quantitative structure-property relationship (QSPR) modeling, Sudhakara et al. [16] investigate the prediction capacity of Degcity indices for the physico-chemical characteristics of polycyclic aromatic hydrocarbons (PAHs). Several methods and results from related research that indicate the effectiveness of numerous indicators in predicting PAH characteristics provide support to this method of prediction [17]. The paper introduces degcity indices, a set of topological indices based on degree-eccentricity, designed to predict the physical properties of chemical compounds, specifically for 67 alkane isomers. The study uses the QSPR method to establish a mathematical model, evaluating the prediction ability of the indices by examining their correlation with physical properties. The research is based on a comprehensive dataset of 67 alkane isomers, providing a robust foundation for analysis.

In our study, we use Non-Steroidal Anti-Inflammatory Drugs (NSAID) as a case study to create QSPR models based on degcity indicators. The study's goal is to demonstrate strong relationships between degcity indexes and the physicochemical features of NSAID medications. Our main contribution is to demonstrate the predictive efficacy of degcity indices for drug-related features, which provides a unique approach to using molecular descriptors in QSPR investigations. This study advances our understanding of NSAID characteristics and shows the use of degcity indices in drug discovery and development, establishing up the possibility for their wider use in computational chemistry. The first application of degcity indices in NSAID modeling is reported, revealing their potential in pharmaceutical chemistry. The research introduces an efficient computational framework for rapid NSAID property prediction, reducing experimental testing. The findings are significant for medicinal chemistry and environmental science, potentially generalizing to other therapeutic classes. In this study, we use five NSAID drugs, viz., Naproxen, Flurbiprofen, Fenoprofen, Ketoprofen, and Ibuprofen, which are considered for analysis. Naproxen and Ibuprofen serves as an anti-inflammatory and analgesic agent, particularly for arthritis and analogous ailments. Its molecular architecture, characterized by aromatic rings and functional groups, is essential for calculating topological indices, which assist in forecasting physicochemical attributes such as solubility and efficacy. Flurbiprofen is useful for decreasing inflammation and treating postoperative ocular irritation. Its structural variety, which includes a fluorine atom and an aromatic scaffold, making it ideal for QSPR experiments that link molecular features to biological activity. Fenoprofen is used to alleviate pain and inflammation caused by arthritis and musculoskeletal conditions. Its biphenyl structure and carboxylic acid group allow for the determination of molecular connectivity and electronegativity indices, which are useful for predicting activity and potency in QSPR models. Ketoprofen is used to treat both acute and chronic pain, such as arthritis. Its keto group and aromatic rings contribute to structural indices associated with molecular reactivity, stability, and pharmacological action in QSPR experiments. The topological index can be derived from its chemical graph. These indices facilitate the prediction of pharmacokinetic properties, including bioavailability, and play a role in QSPR studies. In the present study, we employ the concept of

hydrogen-suppressed molecular graph is a simplified molecular representation in which only non-hydrogen atoms (such as C, O, and N) are represented as nodes and bonds between them as edges, with hydrogens inferred by atomic valency. For instance, ethanol CH_3-CH_2-OH is denoted as (C-C-O). This method is commonly utilized in QSPR/QSAR research and topological index computations (e.g., Zagreb and Wiener indices) to simplify molecular analysis and modeling. It is also used in cheminformatics to do structural comparisons and predictive modeling. While V and E represent vertices and edge sets, respectively, in the chemical graph, the graph $G(V,\ E)$ is thought to be simple, finite, and linked. Eccentricity e_v in a graph is the greatest distance between a vertex and every other vertex in the graph.

$$e_v = max\{d(u,\ v);\ u,\ v \in V\},$$

where $d(u,\ v)$ is a distance between u and v and degree d_v is the number of edges adjacent to a vertex v.

2. Definitions

The recently developed degree-eccentricity related topological indices, called Degcity indices, and are defined as follows [16]:

• First Degcity Indices

$$DC_1^*(G) = \sum_{uv \in E(G)} [e_u + e_v][d_u + d_v]$$

• Second Degcity Indices

$$DC_2^*(G) = \sum_{uv \in E(G)} \frac{[e_u + e_v]}{[d_u + d_v]}$$

• Third Degcity Indices

$$DC_3^*(G) = \sum_{uv \in E(G)} \frac{[d_u + d_v]}{[e_u + e_v]}$$

• Fourth Degcity Indices

$$DC_4^*(G) = \sum_{uv \in E(G)} \sqrt{\frac{[e_u + e_v]}{[d_u + d_v]}}$$

• Fifth Degcity Indices

$$DC_5^*(G) = \sum_{uv \in E(G)} \sqrt{\frac{[d_u + d_v]}{[e_u + e_v]}}$$

• Sixth Degcity Indices

$$DC_6^*(G) = \sum_{uv \in E(G)} \frac{[e_u + e_v]}{[d_u \cdot d_v]}$$

• Seventh Degcity Indices

$$DC_7^*(G) = \sum_{uv \in E(G)} \frac{[d_u + d_v]}{[e_u \cdot e_v]}$$

Where d_u and d_v represent the degree of the vertices u, v and e_u, e_v represent the eccentricity of the vertices $u,\ v$.

3. Results and discussion

This study computes degree-eccentricity-based NSAID drugs indexes. The created indices' QSPR analysis is examined, and it is shown that these indices have a strong correlation with the physicochemical characteristics of the NSAID drugs that are used in the creation of drugs. The five NSAID drugs, viz., Naproxen, Flurbiprofen, Fenoprofen, Ketoprofen, and Ibuprofen, are considered for the analysis. The chem spider was used to obtain the values for these characteristics. Figure 1 displays the molecular structures of several medications. These formations may be considered graphs, in which the bonds between the atoms represent the edges and the atoms themselves represent the vertices.

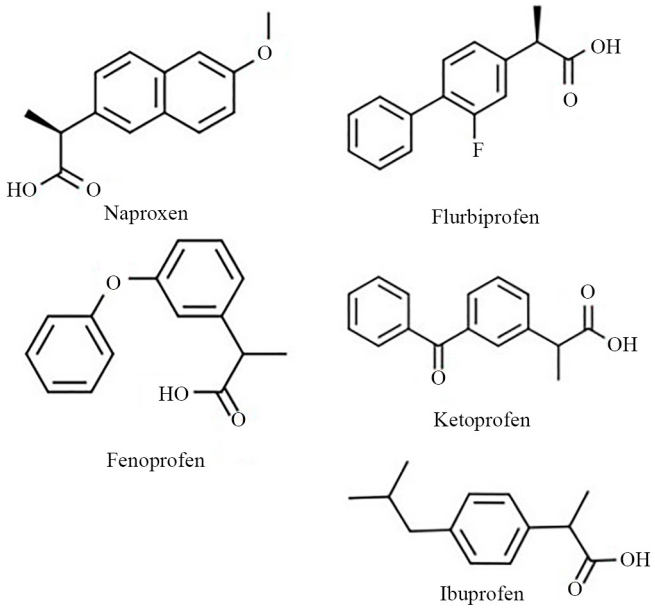

Figure 1. Chemical Structure of NSAID drugs

3.1 *Regression models*

Topological indices are employed to model important physical properties, including molecular weight, boiling point, melting point, complexity, enthalpy, molar refraction, and polarizability.

A simple linear regression describes the relationship between the dependent (or response) variable and the independent variable by analyzing the interaction between two quantitative variables using a linear equation. The physicochemical characteristics of NSAID drugs are regarded as dependent factors, while the degcity indices for the molecular graphs of five different drugs are regarded as independent variables.

The linear regression model used in this work is expressed as:

$$Y = \beta_0 + \beta_1 X. \tag{1}$$

Where Y represent the physicochemical characteristics of drugs, β_0 represent constant, β_1 represent slope and X represents the degcity indices.

We discussed the regression model for the previously described degcity indices, defined as follows, based on the linear regression equation (1):

3.1.1 *Regression models for $DC_1^*(G)$*

$$\text{Molecular Weight} = 0.0853 \cdot [DC_1^*(G)] + 125.6468,$$

$$\text{Boiling Point} = 0.3524 \cdot [DC_1^*(G)] - 146.4384,$$

$$\text{Melting Point} = -0.0257 \cdot [DC_1^*(G)] + 120.8645,$$

$$\text{Complexity} = 0.2045 \cdot [DC_1^*(G)] + 10.1773,$$

$$\text{Enthalpy} = 0.206 \cdot [DC_1^*(G)] + 40.109,$$

$$\text{Molar Refraction} = 0.0185 \cdot [DC_1^*(G)] + 42.9474,$$

$$\text{Polarizability} = 0.0074 \cdot [DC_1^*(G)] + 16.9918.$$

3.1.2 *Regression models for $DC_2^*(G)$*

$$\text{Molecular Weight} = 1.6179 \cdot [DC_2^*(G)] + 137.7182,$$

$$\text{Boiling Point} = 3.8534 \cdot [DC_2^*(G)] + 74.6653,$$

$$\text{Melting Point} = -2.0038 \cdot [DC_2^*(G)] + 208.8641,$$

$$\text{Complexity} = 3.5314 \cdot [DC_2^*(G)] + 60.2391,$$

$$\text{Enthalpy} = 0.331 \cdot [DC_2^*(G)] + 46.6044,$$

$$\text{Molar Refraction} = 0.3434 \cdot [DC_2^*(G)] + 46.0709,$$

$$\text{Polarizability} = 0.1362 \cdot [DC_2^*(G)] + 18.2705.$$

3.1.3 *Regression models for $DC_3^*(G)$*

$$\text{Molecular Weight} = 16.552 \cdot [DC_3^*(G)] + 135.8621,$$

$$\text{Boiling Point} = 234.8905 \cdot [DC_3^*(G)] - 1,106.0631,$$

$$\text{Melting Point} = 86.0967 \cdot [DC_3^*(G)] - 430.3195,$$

$$\text{Complexity} = 56.3725 \cdot [DC_3^*(G)] - 65.643,$$

$$\text{Enthalpy} = 6.0804 \cdot [DC_3^*(G)] + 30.009,$$

$$\text{Molar Refraction} = 3.33 \cdot [DC_3^*(G)] + 46.7805,$$

$$\text{Polarizability} = 1.3538 \cdot [DC_3^*(G)] + 18.3533.$$

3.1.4 *Regression models for $DC_4^*(G)$*

$$\text{Molecular Weight} = 3.7978 \cdot [DC_4^*(G)] + 111.9204,$$

$$\text{Boiling Point} = 10.5314 \cdot [DC_4^*(G)] - 35.1262,$$

$$\text{Melting Point} = -3.9091 \cdot [DC_4^*(G)] + 214.9706,$$

$$\text{Complexity} = 8.4003 \cdot [DC_4^*(G)] + 0.324,$$

$$\text{Enthalpy} = 0.7722 \cdot [DC_4^*(G)] + 41.4781,$$

$$\text{Molar Refraction} = 0.7939 \cdot [DC_4^*(G)] + 40.9933,$$

$$\text{Polarizability} = 0.315 \cdot [DC_4^*(G)] + 16.2519.$$

3.1.5 *Regression models for $DC_5^*(G)$*

$$\text{Molecular Weight} = 25.2699 \cdot [DC_5^*(G)] - 15.7544,$$

$$\text{Boiling Point} = 180.5291 \cdot [DC_5^*(G)] - 1,487.2793,$$

$$\text{Melting Point} = 32.8684 \cdot [DC_5^*(G)] - 238.9664,$$

$$\text{Complexity} = 68.4501 \cdot [DC_5^*(G)] - 406.9074,$$

$$\text{Enthalpy} = 6.8705 \cdot [DC_5^*(G)] - 1.7042,$$

$$\text{Molar Refraction} = 5.3474 \cdot [DC_5^*(G)] + 13.6584,$$

$$\text{Polarizability} = 2.1423 \cdot [DC_5^*(G)] + 5.2024.$$

3.1.6 *Regression models for $DC_6^*(G)$*

$$\text{Molecular Weight} = 0.9457 \cdot [DC_6^*(G)] + 174.1123,$$

$$\text{Boiling Point} = -2.3298 \cdot [DC_6^*(G)] + 458.6414,$$

$$\text{Melting Point} = -3.611 \cdot [DC_6^*(G)] + 322.0821,$$

$$\text{Complexity} = 1.5831 \cdot [DC_6^*(G)] + 170.8871,$$

$$\text{Enthalpy} = 0.1418 \cdot [DC_6^*(G)] + 57.3978,$$

$$\text{Molar Refraction} = 0.2073 \cdot [DC_6^*(G)] + 53.3691,$$

$$\text{Polarizability} = 0.0815 \cdot [DC_6^*(G)] + 21.2143.$$

3.1.7 *Regression models for $DC_7^*(G)$*

$$\text{Molecular Weight} = -4.6025 \cdot [DC_7^*(G)] + 243.6015,$$

$$\text{Boiling Point} = 488.0493 \cdot [DC_7^*(G)] - 554.786,$$

$$\text{Melting Point} = 275.895 \cdot [DC_7^*(G)] - 399.6402,$$

$$\text{Complexity} = 41.4009 \cdot [DC_7^*(G)] + 200.4546,$$

$$\text{Enthalpy} = 5.3399 \cdot [DC_7^*(G)] + 57.1657,$$

$$\text{Molar Refraction} = -1.622 \cdot [DC_7^*(G)] + 69.6857,$$

$$\text{Polarizability} = -0.5606 \cdot [DC_7^*(G)] + 27.4904.$$

3.2 *Comparison of degcity indices with a few physicochemical characteristics' coefficients of correlation and statistical variables*

Table 1 lists the physicochemical characteristics of pharmaceuticals, and Table 2 lists the calculated degcity indices of the medications' molecular structures. Figure 2 displays the graphs of correlation coefficients together with the medications' physicochemical characteristics and degcity indicators. The correlation coefficients of NSAID medicines demonstrate how many parameters, including molecular weight melting point, poarizability, melting point, complexity,

enthalpy and molar refraction are connected. A significant positive correlation indicates that when one attribute rises, so does another. A negative correlation indicates that when one attribute increases, the other reduces. These interactions aid in creating medications with the best potential properties for their intended usage. The association coefficients between medications and their degcity indices using linear regression are shown in Table 3.

Table 1. Physicochemical characteristics of NSAID drugs

Drugs	Molecular weight	Boiling point	Melting point	Complexity	Enthalpy	Molar refraction	Polarizability
Naproxen	230.26	403.9	155	277	69.1	66.5	26.4
Flurbiprofen	244.26	376.2	113	286	65.8	66.6	26.4
Fenoprofen	242.27	169	-	271	66.4	68.4	27.1
Ketoprofen	254.28	431.3	94.7	331	72.4	71.8	28.5
Ibuprofen	206.28	157	76	203	59.3	60.8	24.1

Table 2. Numerical values of indices with NSAID drugs

Drugs	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	1,282	55.109	6.5485	30.0445	10.1388	55.563	1.98
Flurbiprofen	1,322	62.182	6.3791	33.8437	10.2634	61.966	1.888
Fenoprofen	1,408	70.19	5.4388	36.1743	9.737	83.831	1.439
Ketoprofen	1,488	69.8	6.322	36.9169	10.6455	69.607	1.7938
Ibuprofen	940	44.81	5.401	25.6799	8.9236	53.438	1.733

Table 3. Correlation coefficients of physicochemical characteristics of NSAID drugs

Indices	Molecular weight	Boiling point	Melting point	Complexity	Enthalpy	Molar refraction	Polarizability
$DC_1^*(G)$	**0.9731**	0.5553	-0.0945	0.9352	0.8924	**0.9763**	**0.9745**
$DC_2^*(G)$	0.9405	0.3093	-0.3755	0.8225	0.7314	0.9214	0.9158
$DC_3^*(G)$	0.4965	**0.9727**	0.8326	0.6774	0.6933	0.461	0.4696
$DC_4^*(G)$	0.9637	0.369	-0.3198	0.854	0.745	0.9298	0.9246
$DC_5^*(G)$	0.8988	0.8865	0.3769	**0.9754**	**0.929**	0.8778	0.8813
$DC_6^*(G)$	0.633	-0.2153	-0.7792	0.4245	0.3609	0.6404	0.6307
$DC_7^*(G)$	-0.0514	0.7531	**0.9942**	0.1854	0.2269	-0.0837	-0.0725

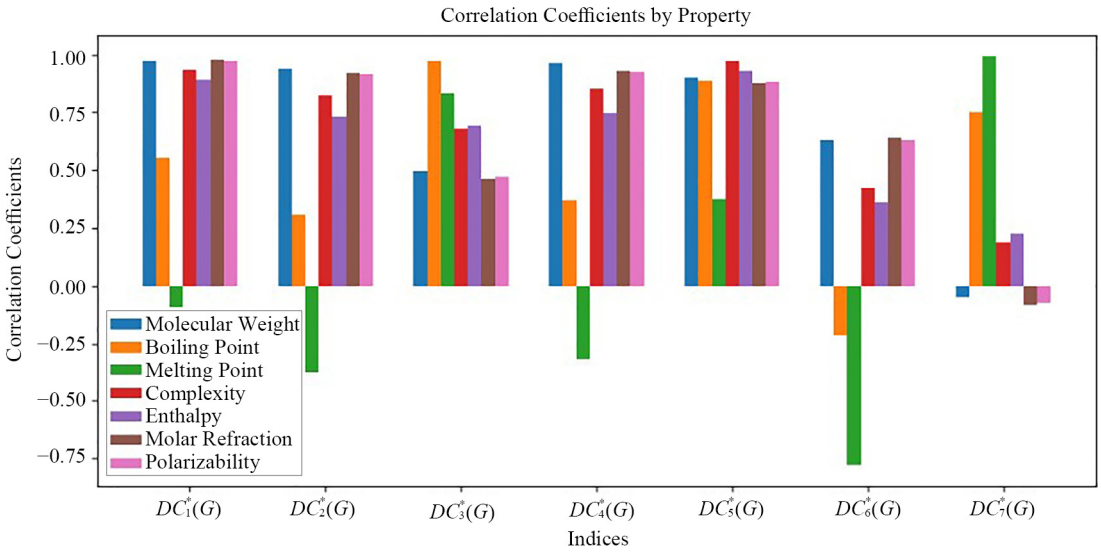

Figure 2. Bar chart shows correlation coefficients for molecular properties across seven indices, with various colors representing each property and displaying the difference in correlation across these indices

Assumed to be near to the theoretical calculations indicated in bold in the table is the coefficient of correlation of the physicochemical characteristics with degcity indices. Model improvements may be determined and comparisons made with this kind of test. The melting point regularly yields a p-value larger than 0.05, except for the $DC_7^*(G)$ indices, suggesting that all attributes that save the melting point are both significant and insignificant. Notably, the r-value is greater than 0.7 and the p-value is less than 0.05. The statistical variables used in the QSPR model of degcity indices are presented in Tables 4-11, which include sample size (N), constant β_0, slope β_1, correlation coefficient (r), coefficient of determination (R^2), fisher's test (F), and significance value (P). In a regression model, R^2 (R-squared) indicates how much of the variance in the dependent variable is explained by the independent variables. The R^2 value goes from 0 to 1, with 1 representing a perfect match and 0 suggesting no explanatory power. The correlation coefficient (r) assesses the degree and direction of a linear link between two variables, with values ranging from -1 (perfect negative correlation) to $+1$ (perfect positive correlation), with 0 signifying no linear relationship. F-statistic, which is used in statistical analysis, particularly regression models, to determine the model's overall significance. It compares explained variance to unexplained variance, with a higher F value suggesting a better model fit. In Table 4, The standard error of estimate (SEE) in QSPR analysis can be calculated using the following formula: $\text{SEE} = \sqrt{\frac{(y_{\text{obs}} - y_{\text{predict}})^2}{n-2}}$. On the other hand, Figure 3 shows the comparison between actual and predicted values of the physicochemical properties of drugs and Tables 12-18 in the supporting data demonstrate a strong correlation between the estimated model values and the real property values and also the comparison of boiling points between estimated and real values using regression models with degcity indices demonstrates the models' accuracy. Estimated values are based on the mathematical link between degcity indices and boiling points, whereas true values are obtained by experimental observations. A restricted correlation between the two suggests that the model can accurately predict boiling points. This validation reveals that degcity indices may properly reflect physicochemical features.

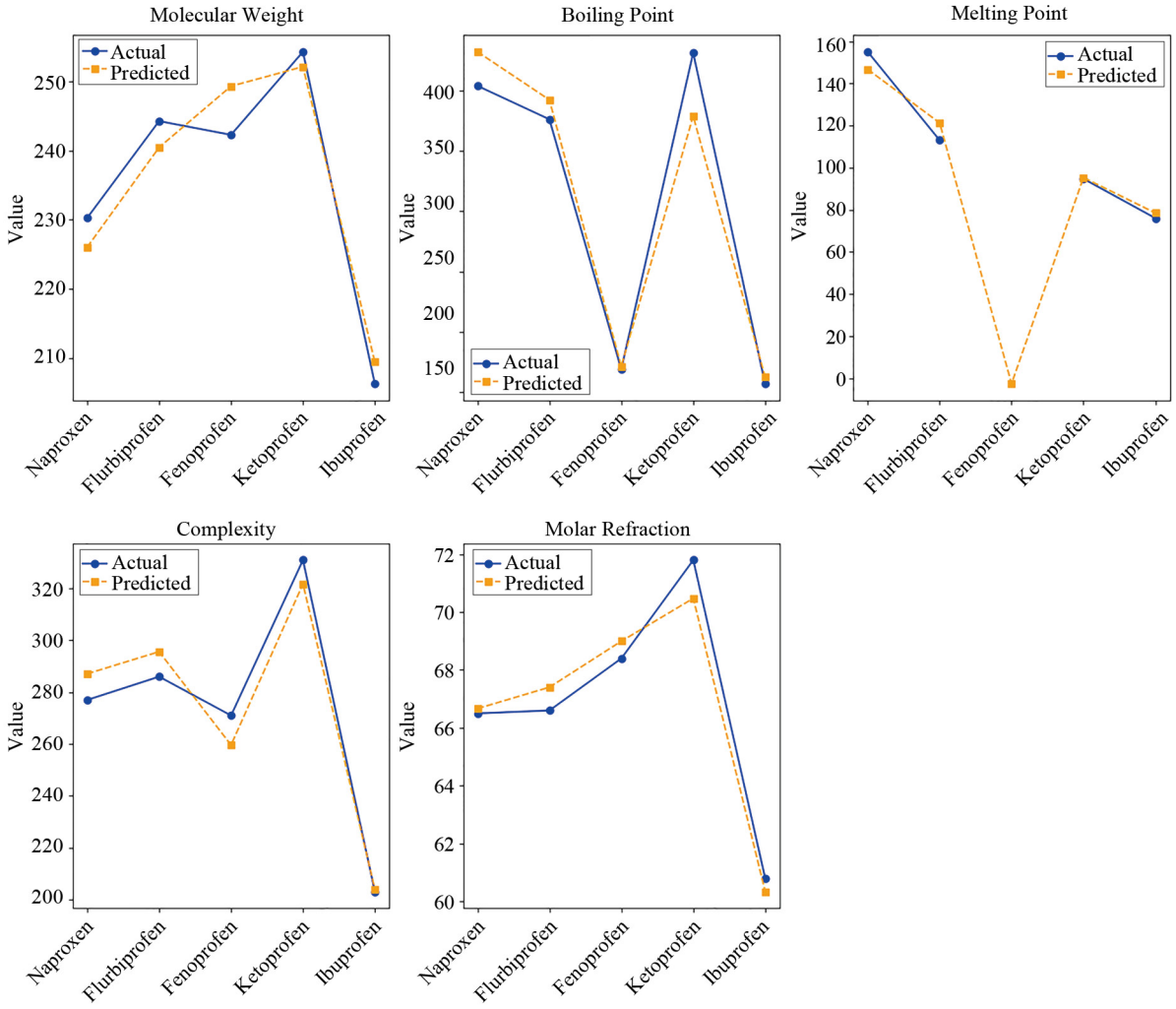

Figure 3. Comparison of actual vs. predicted values for molecular weight, boiling point, melting point, complexity, and molar refraction across five drugs (Naproxen, Flurbiprofen, Fenoprofen, Ketoprofen, and Ibuprofen). The blue circles represent the actual experimental values, while the orange squares represent the predicted values based on linear regression models. Each subplot corresponds to one molecular property, illustrating the alignment between the predicted and actual values for each drug

Table 4. Standard error of estimate for physicochemical characteristics of NSAID drugs

Indices	Molecular weight	Boiling point	Melting point	Complexity	Enthalpy	Molar refraction	Polarizability
$DC_1^*(G)$	4.895	128.1	65.66	18.7992	2.524	0.9978	0.4126
$DC_2^*(G)$	7.2233	146.5	61.1288	30.19	3.814	1.7909	0.7382
$DC_3^*(G)$	18.4587	35.7664	36.535	39.0424	4.031	4.089	1.6231
$DC_4^*(G)$	5.674	143.2	62.49	27.61	3.731	1.6964	0.7003
$DC_5^*(G)$	9.322	71.28	61.09	11.70	2.070	2.207	0.8688
$DC_6^*(G)$	16.46	150.4	41.34	48.06	5.216	3.539	1.427
$DC_7^*(G)$	21.24	101.3	7.100	52.16	5.448	4.591	1.834

Table 5. The linear QSPR models' statistical variables for $DC_1^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	125.6468	0.0853	0.9731	0.947	53.62	0	Significant
Boiling point	5	146.4384	0.3524	0.5553	0.3083	1.337	0.33	Insignificant
Melting point	5	120.8645	0.0257	-0.0945	0.0089	0.027	0.87	Insignificant
Complexity	5	10.1773	0.2045	0.9352	0.8745	20.91	0	Significant
Enthalpy	5	40.109	0.0206	0.8924	0.7964	11.73	0	Significant
Molar refraction	5	42.9474	0.0185	**0.9763**	0.9531	60.97	0	Significant
Polarizability	5	16.9918	0.0074	0.9745	0.9496	56.57	0	Significant

Table 6. The linear QSPR models' statistical variables for $DC_2^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	137.7182	1.6179	**0.9405**	0.8846	23.00	0	Significant
Boiling point	5	74.6653	3.8534	0.3093	0.0956	0.3173	0.61	Insignificant
Melting point	5	208.8641	2.0038	-0.3755	0.141	0.4926	0.53	Insignificant
Complexity	5	60.2391	3.5314	0.8225	0.6765	6.272	0.08	Insignificant
Enthalpy	5	46.6044	0.331	0.7314	0.535	3.451	0.16	Insignificant
Molar refraction	5	46.0709	0.3434	0.9214	0.8489	16.86	0	Significant
Polarizability	5	18.2705	0.1362	0.9158	0.8388	15.61	0	Significant

Table 7. The linear QSPR models' statistical variables for $DC_3^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	135.8621	16.552	0.4965	0.2465	0.9813	0.39	Insignificant
Boiling point	5	1,106.0631	234.8905	**0.9727**	0.9461	52.64	0.33	Significant
Melting point	5	430.3195	86.0967	0.8326	0.6932	6.777	0.08	Insignificant
Complexity	5	65.643	56.3725	0.6774	0.4589	2.544	0.2	Insignificant
Enthalpy	5	30.009	6.0804	0.6933	0.4807	2.777	0.19	Insignificant
Molar refraction	5	46.7805	3.33	0.461	0.2125	0.8095	0.43	Insignificant
Polarizability	5	18.3533	1.3538	0.4696	0.2206	0.8490	0.42	Insignificant

Table 8. The linear QSPR models' statistical variables for $DC_4^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	111.9204	3.7978	**0.9637**	0.9288	39.13	0	Significant
Boiling point	5	35.1262	0.5314	0.369	0.1361	0.4727	0.54	Insignificant
Melting point	5	214.9706	3.9091	-0.3198	0.1023	0.3418	0.59	Insignificant
Complexity	5	0.324	8.4003	0.854	0.7294	8.085	0.06	Insignificant
Enthalpy	5	41.4781	0.7722	0.745	0.555	3.741	0.14	Insignificant
Molar refraction	5	40.9933	0.7939	0.9298	0.8645	19.13	0	Significant
Polarizability	5	16.2519	0.315	0.9246	0.8549	17.67	0	Significant

Table 9. Statistical parameters for the linear QSPR model for $DC_5^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	15.7544	25.2699	0.8988	0.8078	12.61	0	Significant
Boiling point	5	1,487.279	180.5291	0.8865	0.7858	11.01	0	Significant
Melting point	5	238.9664	32.8684	0.3769	0.1421	0.4967	0.53	Insignificant
Complexity	5	406.9074	68.4501	**0.9754**	0.9514	58.76	0	Significant
Enthalpy	5	1.7042	6.8705	0.929	0.8631	18.91	0	Significant
Molar refraction	5	13.6584	5.3474	0.8778	0.7705	10.07	0	Significant
Polarizability	5	5.2024	2.1423	0.8813	0.7767	10.43	0	Significant

Table 10. The linear QSPR models' statistical variables for $DC_6^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	174.1123	0.9457	0.633	0.4007	2.005	0.25	Insignificant
Boiling point	5	458.6414	2.3298	-0.2153	0.0463	0.1458	0.72	Insignificant
Melting point	5	322.0821	3.611	-0.7792	0.6072	4.637	0.12	Insignificant
Complexity	5	170.8871	1.5831	0.4245	0.1802	0.6595	0.47	Insignificant
Enthalpy	5	0.1418	57.3978	0.3609	0.1302	0.4492	0.55	Insignificant
Molar refraction	5	0.2073	53.3691	0.6404	0.4101	2.086	0.24	Insignificant
Polarizability	5	21.2143	0.0815	0.6307	0.3978	1.981	0.25	Insignificant

Table 11. The linear QSPR models' statistical variables for $DC_7^*(G)$

Property	N	β_0	β_1	r	R^2	F	P	Indicator
Molecular weight	5	243.6015	4.6025	-0.0514	0.0026	0.0079	0.93	Insignificant
Boiling point	5	554.786	488.049	0.7531	0.5672	3.931	0.14	Insignificant
Melting point	5	399.64	275.895	**0.9942**	0.9884	255.9	0	Significant
Complexity	5	200.4546	41.4009	0.1854	0.0344	0.1068	0.76	Insignificant
Enthalpy	5	57.1657	5.3399	0.2269	0.0515	0.1628	0.71	Insignificant
Molar refraction	5	69.6857	1.622	-0.0837	0.007	0.02115	0.89	Insignificant
Polarizability	5	27.4904	0.5606	-0.0725	0.0053	0.0158	0.90	Insignificant

Table 12. Comparison of the molecular weight estimated and real values from the regression models of the degcity indices

Drugs	Molecular weight	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	230.26	235	226.88	244.25	226	240.4	226.66	234.5
Flurbiprofen	244.26	238.4	238.322	241.45	240.45	243.6	232.7	234.9
Fenoprofen	242.27	245.7	251.28	225.89	249.3	230.29	253.4	236.98
Ketoprofen	254.28	252.6	250.648	240.5038	252.1	253.26	239.94	235.3
Ibuprofen	206.28	205.83	210.216	225.26	209.45	209.74	224.65	235.6

Table 13. Comparison of boiling point estimated and real values from the regression models of the degcity indices

Drugs	Boiling point	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	403.9	305.34	287	432.1	281.28	343.07	329.19	411.5
Flurbiprofen	376	319.43	314.3	392.33	321.29	365.29	314.27	366.65
Fenoprofen	169	349.74	345.13	171.46	345.84	345.84	263.33	147.52
Ketoprofen	431.3	377.93	343.63	378.9	353.66	353.66	296.47	323.1
Ibuprofen	157	184.82	247.34	162.58	235.32	235.32	334.14	291

Table 14. Comparison of the melting point estimated and real values from the regression models of the degcity indices

Drugs	Melting point	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	155	87.9171	98.44	133.48	97.52	94.28	121.44	146.63
Flurbiprofen	113	86.89	84.26	118.89	82.67	98.37	98.32	121.25
Fenoprofen	0	84.68	68.22	37.94	73.56	81.07	19.37	-2.627
Ketoprofen	95	82.62	68.99	113.94	70.66	110.93	70.73	96.64
Ibuprofen	76	96.71	119.07	34.69	114.58	54.34	129.12	78.48

Table 15. Comparison of the complexity estimated and real values from the regression models of the degcity indices

Drugs	Complexity	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	277	272.35	253.89	303.51	252.71	287.09	255.95	282.43
Flurbiprofen	286	280.53	278.75	293.96	284.62	295.62	265.76	278.62
Fenoprofen	271	298.1	306.89	240.95	304.19	259.62	299.23	260.03
Ketoprofen	331	314.47	305.52	290.74	310.44	321.78	277.45	274.93
Ibuprofen	203	202.4	1 217.7	238.82	216.04	203.91	252.7	272.2

Table 16. Comparison of the enthalpy estimated and real values from the regression models of the degcity indices

Drugs	Enthalpy	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	69.1	66.52	64.84	69.82	64.68	67.95	65.28	67.74
Flurbiprofen	65.8	67.34	67.19	68.79	67.612	68.81	66.18	67.25
Fenoprofen	66.4	69.11	69.84	63.08	69.41	65.19	69.28	64.85
Ketoprofen	72.4	70.76	69.71	68.45	69.98	71.44	67.27	66.77
Ibuprofen	59.3	59.473	61.44	62.85	61.308	59.605	64.975	66.419

Table 17. Comparison of the molar refraction estimated and real values from the regression models of the degcity indices

Drugs	Molar refraction	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	66.5	66.66	64.99	68.59	64.85	67.87	64.89	66.47
Flurbiprofen	66.6	67.4	67.42	68.02	67.86	68.54	66.21	66.623
Fenoprofen	68.4	68.99	70.17	64.89	69.71	65.73	70.75	67.352
Ketoprofen	71.8	70.47	70.04	67.83	70.3	70.58	67.79	66.77
Ibuprofen	60.8	60.34	61.46	64.76	61.38	61.38	64.45	66.87

Table 18. Comparison of the polarizability estimated and real values from the regression models of the degcity indices

Drugs	Polari-zability	$DC_1^*(G)$	$DC_2^*(G)$	$DC_3^*(G)$	$DC_4^*(G)$	$DC_5^*(G)$	$DC_6^*(G)$	$DC_7^*(G)$
Naproxen	26.4	26.48	35.69	27.22	25.72	26.92	25.74	26.38
Flurbiprofen	26.4	26.77	37.93	26.99	26.91	27.19	26.26	26.43
Fenoprofen	27.1	27.41	40.46	25.72	27.65	26.06	28.05	26.68
Ketoprofen	28.5	28.003	40.34	26.91	27.88	28.01	26.89	26.48
Ibuprofen	24.1	23.95	32.44	25.66	24.34	24.32	25.57	26.52

4. Conclusion

In this work, we use degcity indices obtained from the chemical graphs of NSAIDs to build a QSPR model for them. The physicochemical characteristics of the NSAIDs and the chosen topological indices are quantitatively correlated by the predicted QSPR model. The predictive effectiveness of our model is confirmed, suggesting that it may be a helpful tool for guiding NSAID drug development initiatives. The $DC_2^*(G)$ and $DC_4^*(G)$ indices of the chemical graphs of medicines exhibit the most significant values of correlation for molecular weight, with r = 0.9405 and r = 0.9637, based on the statistical variables and degcity indices utilized in the linear QSPR model. For molar refraction, the $DC_1^*(G)$ index reaches its greatest correlation value at r = 0.9763. At r = 0.9727, the boiling point has the strongest correlation value for the $DC_3^*(G)$ index. The melting point has the greatest correlation value (r = 0.9942) for the $DC_7^*(G)$ index, whereas complexity has the largest correlation value (r = 0.9754) for the $DC_5^*(G)$ index. These findings offer a theoretical and financially viable foundation for the development of novel medications with comparable architectures for enhanced therapeutic effects. Researchers in the pharmaceutical sciences may find the information in this study useful in extrapolating the physicochemical characteristics of new NSAID medication designs to improve therapeutic effectiveness. Our technique improves predicted accuracy (better R^2, lower RMSE) compared to existing models, particularly for NSAIDs with similar structural patterns. It has benefits like as simplicity, minimal computing cost, and consistent predictions across varied datasets. However, it has limits with complicated structures and requires precise molecular graph representations.

Conflict of interest

The authors declare no competing financial interest.

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