scientific reports

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Quantitative structure property relationship and multiattribute decision analysis of antianginal drugs using topological indices

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Angina is a condition characterized by chest pain or discomfort due to insufficient blood flow to the heart muscle. Effective management focuses on reducing symptoms and preventing disease progression through lifestyle modifications, medications, and interventional procedures. Timely diagnosis and treatment are crucial for enhancing patient quality of life. Designing and developing experimental drugs is challenging and costly, which makes mathematical and computational methods essential for efficient drug discovery. In this article, we introduce a novel molecular descriptor based on a graph theory-driven degree partitioning technique, integrated into a quantitative structure-property relationships (QSPR) framework. Using quadratic regression, we determine the optimal predictors for four key properties boiling point, enthalpy of vaporization, flash point, and index of refraction for sixteen anti-angina drugs based on nine degree-based topological indices. Furthermore, by combining these descriptors with the multi-attribute decision-making additive ratio assessment technique, we achieve robust and reliable drug rankings. Our innovative integration of a new molecular descriptor with advanced statistical and decision-making methods not only improves predictive accuracy but also provides a novel and efficient approach for the development and optimization of angina drug therapies.

Keywords Angina disease, Molecular graph, QSPR analysis, Regression model, ARASS method

Graph theoretical applications in chemistry have increased significantly in the recent years. Chemical graph theory is a branch of mathematical chemistry based on topology and applies graph theory to the mathematical explanation of chemical procedures. In many areas of chemistry, graphs play an important part in the modeling of chemical compounds through the use of molecular structure. A molecular descriptor offers a more precise mathematical representation of a possible molecular structure. Molecular descriptors that are most frequently utilized are chemical bonding indices. The term topological indices is commonly utilized to characterize these chemical bonds. Since the concepts behind topological indices are derived from the concepts of graph theory, these are viewed as graph invariants. These molecular descriptors can be distance, degree, and neighborhood-based, as discussed by Balaban[1]; Gutman[2]; Mondal et al.[3].

To create novel medications, research is constantly conducted to treat angina patients and cure the illness. Although the procedure of designing and developing experimental drugs is expensive, time-consuming, and difficult. Mathematical and computational methods are crucial to accomplishing this objective in the best possible way. Topological indices: one of these computational and mathematical methods is widely employed in the medications utilized to treat different diseases. The topological index is a useful part or the result of specific standardized tests that are produced through a logical and computational method that transforms the chemical data given within a graphical representation of a molecules, as explained by Arockiaraj et al.[4] and Paul et al.[5].

The rising resistance of angina to existing medical treatments has discovered novel angina drugs as a significant topic to study in pharmaceutical research. QSPR modeling is essential for forecasting the biological impact of these medications based on the molecules. Using topological descriptors, which summarize the molecular structure in terms of connectivity and can significantly simplify drug property estimation is a crucial

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component of QSPR modeling. Imani et al.[6] examined the quantitative structure activity relationship modeling of molecular properties for alzheimers disease using random forest. Abubakar et al.[7] evaluated the QSPR analysis of 15 antituberculosis medicines using support vector regression and computed the neighborhood degree-based topological indices of these medications. Support vector regressions effectiveness was calculated by comparing it with classical linear regression. Awan et al.[8] explained the topological indices and linear regression models of various compounds with potential antimalarial compounds, including quinine, primaquine, artemether, artelinic acid, modified triazoles, and others. Different beta-blockers used to treat cardiac disease and computed degree-based topological indices for each based on the M-polynomial were explored by Hasani and Ghods[9]. Kirana et al.[10] analyzed Quinolone antibiotics using curvilinear regression models and the computation of eleven topological indices through QSPR analysis. The application of topological indices for estimating the usefulness of various medications utilized to treat blood cancer was the main objective of Zhang et al.[11]. For a family of benzenoid hydrocarbon molecules, Ravi and Desikan[12] computed the reduced reverse degree based indices in the QSPR analysis. Hui et al.[13] utilized topological descriptors as independent variables in both linear and multiple regression models to assess the chemical and physical properties of antiemetic medications. Degree-based topological descriptors and curvilinear regression models for thirteen skin cancer medications were analyzed by Khan et al.[14].

An essential field of decision science that deals with difficult decision issues involving several different factors is multi-attribute decision-making. This method is crucial in scenarios where judgments cannot be made using a single criterion and substitutes for taking into consideration many variables to get a reasonable result. Applications of multi-attribute decision-making are found in many fields, such as public policy, engineering, business, and healthcare, where decisions frequently have important and far-reaching effects. For example, in the healthcare industry, multi-attribute decision-making can help choose the best course of action by weighing patient preferences, expenses, adverse reactions, and efficient implementation. The additive ratio assessment technique eliminates the influence of different measurement units and simplifies complex decision-making problems by using a relative indicator (utility degree) to identify the best alternative. This indicator can indicate the differences between the alternatives and the optimal solution. Zavadskas and Turskis[15] introduced the additive ratio assessment method in 2010. Junior et al.[16] developed a decision support system that used the additive ratio assessment method to calculate criteria, sub-criteria, and alternative assessment data to provide appropriate housing for potential purchasers. Arshad[17] utilized the additive ratio assessment and entropy methodologies to help decision-makers evaluate potential warehouse locations that best satisfy the organizations operational and strategic goals. To determine a final ranking of company assessment data on supplier services, Wahyudi[18] purposed to measure the extent of company experience with supplier services by applying the additive ratio assessment approach.

Recent advances in molecular descriptor development have significantly contributed to the field of QSPR modeling. For instance, innovative descriptor optimization techniques have enhanced the prediction of chemical properties[30,31]. Other recent works have successfully integrated graph theory-based methodologies to capture complex molecular topologies, thereby improving model accuracy[32,33]. Furthermore, the potential of degree partitioning techniques in representing finite graphs has been underscored in contemporary research[34–38]. In our study, we build on these developments by introducing a new molecular descriptor based on a graph theory-based degree partitioning technique, which provides a robust and efficient representation of molecular topology. Comparative analysis with these recent studies confirms the enhanced predictive performance and novelty of our approach in the context of anti-angina drug evaluation.

Motivation

We used nine degree based topological indices to develop the QSPR model and evaluated the physiochemical properties of sixteen different medications. For the first time, angina drugs are being studied using degree based topological indices. We emphasize the importance of selecting medications for treating angina with prioritization based on factors such as patient preferences, cost-effectiveness, efficacy, safety, and accessibility. The results of the study may help determine which drug is most effective for helping angina patients in managing their symptoms, improving their quality of life, and taking better care of their illness. This study also identify the best-ranked angina medications that have not been previously studied.

Contribution

The following points summarize our work contribution to this study:

- There are nine topological indices and sixteen drug structures. By comparing topological indices with four physicochemical properties of the medications, QSPR models were developed to evaluate reliability. The computation procedure is carried out for angina drugs such as Acebutolol, Ranolazine, Metoprolol, Amlodipine, Atenolol, Carvedilol, Nitroglycerin, Nadolol, Amyl nitrite, Nicorandil, Propranolol, Molsidomine, Nicardipine, Nifedipine, Diltiazem, and Ivabradine. Then, using linear and quadratic regression analysis, the obtained values are assessed through QSPR modeling to investigate different physicochemical properties of the medications, including boiling point, enthalpy of vaporization, flash point, and index of refraction.
- The analysis of the graphical data is conducted using Microsoft Excel and Matlab to make a graph.
- We examined the relationship between the rankings produced by the multi-attribute decision-making technique and the computed topological indices.

Basic definitions

The structure of the medications is represented as a network known as a molecular graph, where every vertex represents an atom and every edge represents a chemical bond between the atoms, to compute topological indices. Consider a molecular graph G = (V, E) with vertex set V(G) and edge set E(G). In graph G, the numbers |V(G)| and |E(G)| stand for the number of vertices and edges, respectively. The degree of vertex u ∈ V(G) is expressed

by deg(u) or d(u) and is the number of vertices that are adjacent to u. The expression e = uv, where e ∈ E(G), represents the edge between the vertices u and v. Hydrogen atoms are often not included in chemical graphs because they have a valence of one since they only make one bond in many organic molecules, as presented by Kirmani et al.[19]. The following degree-based topological indices are utilized in this paper:

First and second Zagreb index

The Zagreb indices developed by Das and Gutman[20], Gutman and Trinajstić[21] and Gutman et al.[22]:

$$M_1(G) = \sum_{uv \in E(G)} [d_u + d_v].$$

$$M_2(G) = \sum_{uv \in E(G)} [d_u . d_v].$$

Harmonic index

Fajtlowicz[23] was the one who initially introduced the harmonic index.

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

Forgotten index

The forgotten topological index was introduced by Furtula and Gutman[24] in 2015.

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

Inverse sum indeg index

The inverse sum index was presented by Vukičević and Gašperov[25] in 2010. Extreme inverse sum index values were discovered in 2015 by Sedlar et al.[26] for various kinds of graph types, such as chemical trees, connected graphs, molecular graphs, and trees. The inverse sum index is defined as follows:

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

Augmented Zagreb index

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3.$$

Atom bond connectivity index

Estrada et al.[27] created the degree-based topological index atom bond connectivity index, which is defined as follows:

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

Hyper Zagreb index

An enhanced form of the Zagreb index, the hyper Zagreb index was proposed by Shirdel et al.[28] in 2013. The hyper Zagreb index formula is defined as follows:

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

Geometric arithmetic index

Vukicevic and Furtula[29] described the geometric arithmetic index in 2009. The geometric arithmetic index has the following computational definition:

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

Methods and materials

In this section, we evaluate the topological indices of angina drugs. We analyze sixteen drugs: Acebutolol, Ranolazine, Metoprolol, Amlodipine, Atenolol, Carvedilol, Nitroglycerin, Nadolol, Amyl nitrite, Nicorandil,

Drugs Name	$M_1(G)$	$M_2(G)$	H(G)	F(G)	ISI(G)	AZI(G)	ABC(G)	HM(G)	GA(G)
Acebutolol	110	120	10.7333	276	25.3667	171.0313	17.5460	516	22.9167
Ranolazine	154	175	14.4667	384	36.5667	255.6719	23.6508	734	32.0634
Metoprolol	80	85	8.2667	192	18.7176	130.125	13.0561	362	17.3590
Amlodipine	136	160	12.9667	346	32.4	240.625	20.6201	666	28.1511
Atenolol	86	91	8.5	212	19.75	128.875	13.9820	394	18.1281
Carvedilol	154	180	14.5333	378	37.5167	276.3281	23.2417	738	32.5462
Nitroglycerin	62	62	6.4	154	13.7	84.25	10.5558	278	13.0749
Nadolol	112	126	9.6333	304	25.2833	163.4080	16.9471	556	21.7590
Amyl nitrite	28	26	3.5667	62	6.3667	46.75	5.1685	62	6.6547
Nicorandil	66	70	6.9333	156	15.55	109.5156	10.8943	296	14.5173
Propranolol	92	103	8.8667	226	21.85	152.9063	14.3894	432	19.4364
Molsidomine	82	92	8.1	198	19.7167	142.7656	12.7969	382	17.6270
Nicardipine	176	205	16.0333	452	41.5167	290.75	26.6052	862	35.7423
Nifedipine	126	151	11.2333	334	29.5333	210.7656	18.6772	636	24.9605
Diltiazem	148	173	13.3667	380	35.0167	245.2188	22.2246	726	30.0103
Ivabradine	186	223	16.1857	496	43.8476	311.8975	26.9839	942	36.7746

Table 1. Sixteen angina drugs and the values of nine topological indices.

Drugs name	$\mathcal{BP}$ (°C)	$\mathcal{EV}$ (kJ/mol)	$\mathcal{FP}$ (°C)	$\mathcal{IR}$
Acebutolol	564.1	89.2	295.0	1.543
Ranolazine	624.1	97.2	331.2	1.586
Metoprolol	398.6	68.5	194.9	1.508
Amlodipine	527.2	80.2	272.6	1.546
Atenolol	508.0	81.9	261.1	1.540
Carvedilol	655.2	101.4	350.1	1.657
Nitroglycerin	295.8	51.4	145.7	1.489
Nadolol	526.4	84.3	272.2	1.574
Amyl nitrite	99.1	32.4	10.0	1.425
Nicorandil	456.7	71.7	230.0	1.548
Propranolol	434.9	72.8	216.8	1.581
Molsidomine	354.8	60.0	168.4	1.606
Nicardipine	603.4	89.8	318.7	1.582
Nifedipine	475.3	73.9	241.2	1.559
Diltiazem	594.4	88.6	313.3	1.621
Ivabradine	626.9	92.8	332.9	1.560

Table 2. Sixteen angina drugs and their physicochemical properties.

Propranolol, Molsidomine, Nicardipine, Nifedipine, Diltiazem, and Ivabradine. The values of the topological indices shown in Table 1 are calculated using the described mathematical techniques. The data in Table 2 are obtained from ChemSpider. Fig 1 displays the corresponding drug structures. Additionally, we evaluated various topological indices, including the first and second Zagreb index, harmonic index, forgotten index, inverse sum indeg index, augmented index, atom-bond connectivity index, hyper Zagreb index, and geometric arithmetic index, based on the physicochemical properties of angina medications. These properties include boiling point ($\mathcal{BP}$), enthalpy of vaporization ($\mathcal{EV}$), flash point ($\mathcal{FP}$), and index of refraction ($\mathcal{IR}$). We utilized analytical approaches, edge partition techniques, degree-counting processes, and theoretical graph utilities to complete the mathematical computations. ChemDraw software is a useful tool for drawing chemical structures in two dimensions. Microsoft Excel and Matlab are effective tools for constructing line or correlation graphs. Matlab is used to create 2D graphs that compare topological indices and drug properties.

Regression models

A regression model is a statistical method used to estimate the relationships between a dependent variable and one or more independent variables. It can be used to predict the future strength of the relationship between variables and to measure the degree of that relationship. A linear regression model is used to predict the value of one variable depending on the value of another variable. The factors we used to predict the value of the dependent variable are known as independent or explanatory variables, while the variable we seek to forecast is

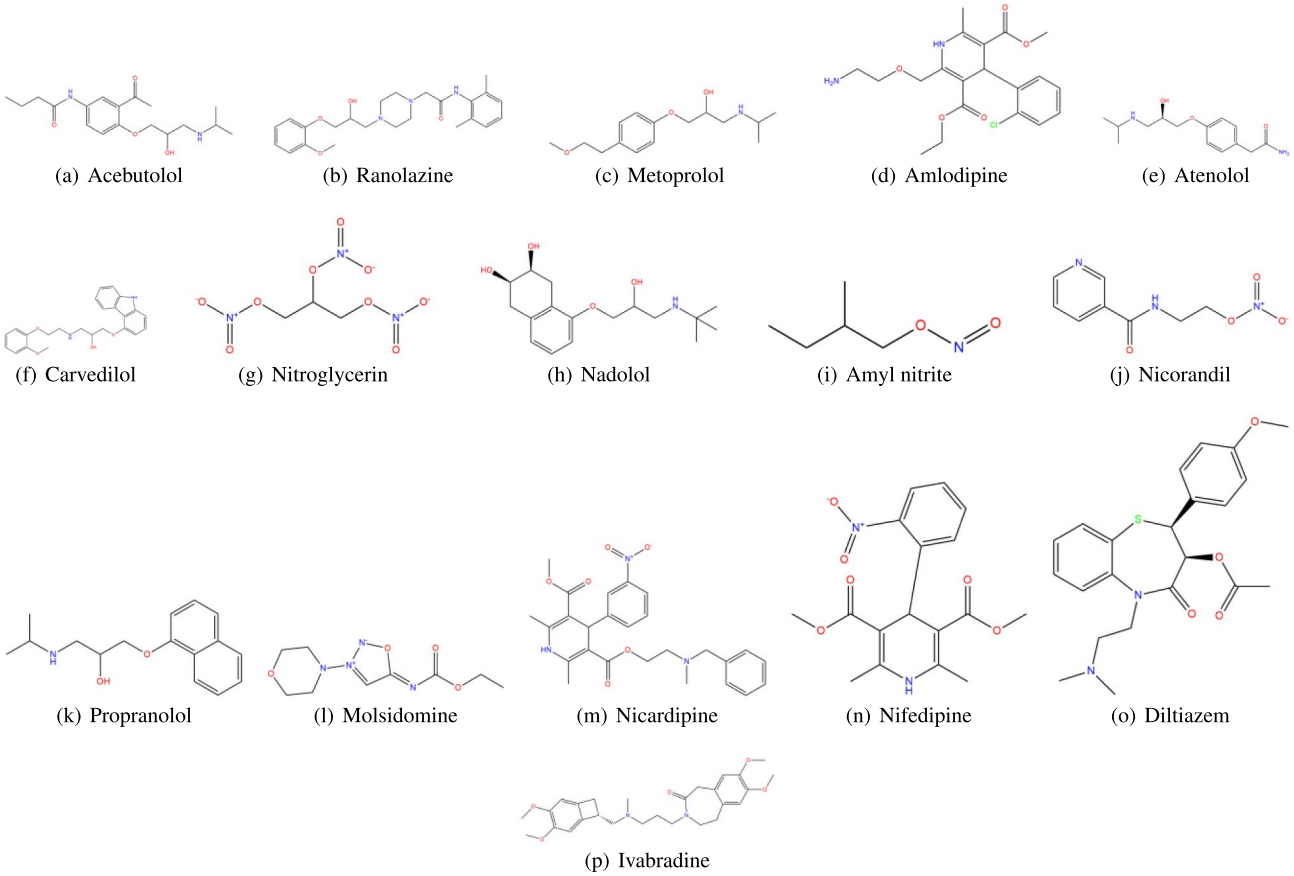


Fig. 1. Chemical structures of the drugs that help fight angina disease.

known as the dependent variable. This model assumes that the relationship is linear, meaning that changes in the independent variables produce proportional changes in the dependent variable. A quadratic regression model is used when the relationship between the variables is expected to be curved rather than linear. This model fits a parabolic curve to the data by incorporating squared terms of the independent variables, allowing it to capture more complex, non-linear relationships. In this section, we examined the connection between computed topological indices and physicochemical properties using regression models. We summarized the calculations of topological indices and physicochemical properties of molecular structures in Table 1 and Table 2, respectively. The resulting values can be used to develop regression models. To establish a connection between the dependent and independent variables, we have two regression models for each considered property. For these models, we typically have an equation.

$$X = B(Y_i) + A$$

$$X = C(Y_i)^2 + B(Y_i) + A$$

where X is dependent variable, Y_i(i = 1, 2, 3,...) are independent variables, A is the regression model constant, and B and C are the coefficients for descriptor.

First Zagreb index

Linear regression

$$\mathcal{BP} = 2.8813[\mathrm{M}_1(\mathrm{G})] + 160.267$$
$$\mathcal{EV} = 0.345[\mathrm{M}_1(\mathrm{G})] + 38.4867$$
$$\mathcal{FP} = 1.7309[\mathrm{M}_1(\mathrm{G})] + 52.6224$$
$$\mathcal{IR} = 0.0008141[\mathrm{M}_1(\mathrm{G})] + 1.4663$$

Quadratic regression

$$\mathcal{BP} = -0.0220[\mathrm{M}_1(\mathrm{G})]^2 + 7.785[\mathrm{M}_1(\mathrm{G})] - 71.9402$$
$$\mathcal{EV} = -0.0028[\mathrm{M}_1(\mathrm{G})]^2 + 0.9697[\mathrm{M}_1(\mathrm{G})] + 8.9052$$
$$\mathcal{FP} = -0.0135[\mathrm{M}_1(\mathrm{G})]^2 + 4.7389[\mathrm{M}_1(\mathrm{G})] - 89.8173$$
$$\mathcal{IR} = 0.0000[\mathrm{M}_1(\mathrm{G})]^2 + 0.0033[\mathrm{M}_1(\mathrm{G})] + 1.3473$$

Second Zagreb index

Linear regression

$$\mathcal{BP} = 2.2579[\mathrm{M}_2(\mathrm{G})] + 195.8964$$
$$\mathcal{EV} = 0.2693[\mathrm{M}_2(\mathrm{G})] + 42.891$$
$$\mathcal{FP} = 1.3551[\mathrm{M}_2(\mathrm{G})] + 74.1823$$
$$\mathcal{IR} = 0.0006473[\mathrm{M}_2(\mathrm{G})] + 1.4752$$

Quadratic regression

$$\mathcal{BP} = -0.0150[\mathrm{M}_2(\mathrm{G})]^2 + 6.0844[\mathrm{M}_2(\mathrm{G})] - 4.708$$
$$\mathcal{EV} = -0.0019[\mathrm{M}_2(\mathrm{G})]^2 + 0.7634[\mathrm{M}_2(\mathrm{G})] + 16.9859$$
$$\mathcal{FP} = -0.0091[\mathrm{M}_2(\mathrm{G})]^2 + 3.6873[\mathrm{M}_2(\mathrm{G})] - 48.0778$$
$$\mathcal{IR} = 0.0000[\mathrm{M}_2(\mathrm{G})]^2 + 0.0027[\mathrm{M}_2(\mathrm{G})] + 1.3698$$

Harmonic index

Linear regression

$$\mathcal{BP} = 34.9958[\mathrm{H}(\mathrm{G})] + 112.6942$$
$$\mathcal{EV} = 4.2065[\mathrm{H}(\mathrm{G})] + 32.6182$$
$$\mathcal{FP} = 21.0229[\mathrm{H}(\mathrm{G})] + 24.0447$$
$$\mathcal{IR} = 0.009857[\mathrm{H}(\mathrm{G})] + 1.4532$$

Quadratic regression

$$\mathcal{BP} = -3.2839[\mathrm{H}(\mathrm{G})]^2 + 104.1444[\mathrm{H}(\mathrm{G})] - 209.1402$$
$$\mathcal{EV} = -0.4077[\mathrm{H}(\mathrm{G})]^2 + 12.7911[\mathrm{H}(\mathrm{G})] - 7.3365$$
$$\mathcal{FP} = -2.0149[\mathrm{H}(\mathrm{G})]^2 + 63.45[\mathrm{H}(\mathrm{G})] - 173.4218$$
$$\mathcal{IR} = -0.0016[\mathrm{H}(\mathrm{G})]^2 + 0.0433[\mathrm{H}(\mathrm{G})] + 1.2977$$

Forgotten index

Linear regression

$$\mathcal{BP} = 1.0558[\mathrm{F}(\mathrm{G})] + 183.8097$$
$$\mathcal{EV} = 0.1259[\mathrm{F}(\mathrm{G})] + 41.4652$$
$$\mathcal{FP} = 0.6344[\mathrm{F}(\mathrm{G})] + 66.7236$$
$$\mathcal{IR} = 0.000291[\mathrm{F}(\mathrm{G})] + 1.4751$$

Quadratic regression

$$\mathcal{BP} = -0.0031[\mathrm{F}(\mathrm{G})]^2 + 2.8319[\mathrm{F}(\mathrm{G})] - 26.5146$$
$$\mathcal{EV} = -0.0004[\mathrm{F}(\mathrm{G})]^2 + 0.3563[\mathrm{F}(\mathrm{G})] + 14.1782$$
$$\mathcal{FP} = -0.0019[\mathrm{F}(\mathrm{G})]^2 + 1.724[\mathrm{F}(\mathrm{G})] - 62.3027$$
$$\mathcal{IR} = 0.0000[\mathrm{F}(\mathrm{G})]^2 + 0.0012[\mathrm{F}(\mathrm{G})] + 1.3653$$

Inverse sum indeg index

Linear regression

$$\mathcal{BP} = 11.9335[\mathrm{ISI}(\mathrm{G})] + 168.7892$$
$$\mathcal{EV} = 1.4302[\mathrm{ISI}(\mathrm{G})] + 39.4728$$
$$\mathcal{FP} = 7.1637[\mathrm{ISI}(\mathrm{G})] + 57.8769$$
$$\mathcal{IR} = 0.003456[\mathrm{ISI}(\mathrm{G})] + 1.4665$$

Quadratic regression

$$\mathcal{BP} = -0.3874[\mathrm{ISI(G)}]^2 + 32.2857[\mathrm{ISI(G)}] - 56.5686$$
$$\mathcal{EV} = -0.0490[\mathrm{ISI(G)}]^2 + 4.0046[\mathrm{ISI(G)}] + 10.967$$
$$\mathcal{FP} = -0.2365[\mathrm{ISI(G)}]^2 + 19.59[\mathrm{ISI(G)}] - 79.7183$$
$$\mathcal{IR} = -0.0002[\mathrm{ISI(G)}]^2 + 0.0139[\mathrm{ISI(G)}] + 1.3514$$

Augmented Zagreb index

Linear regression

$$\mathcal{BP} = 1.5949[\mathrm{AZI(G)}] + 188.9077$$
$$\mathcal{EV} = 0.1908[\mathrm{AZI(G)}] + 41.9405$$
$$\mathcal{FP} = 0.9558[\mathrm{AZI(G)}] + 70.2513$$
$$\mathcal{IR} = 0.0004742[\mathrm{AZI(G)}] + 1.4701$$

Quadratic regression

$$\mathcal{BP} = -0.0079[\mathrm{AZI(G)}]^2 + 4.5234[\mathrm{AZI(G)}] - 37.8644$$
$$\mathcal{EV} = -0.0010[\mathrm{AZI(G)}]^2 + 0.5618[\mathrm{AZI(G)}] + 13.214$$
$$\mathcal{FP} = -0.0047[\mathrm{AZI(G)}]^2 + 2.7209[\mathrm{AZI(G)}] - 66.4361$$
$$\mathcal{IR} = 0.0000[\mathrm{AZI(G)}]^2 + 0.002[\mathrm{AZI(G)}] + 1.3522$$

Atom bond connectivity index

Linear regression

$$\mathcal{BP} = 20.8665[\mathrm{ABC(G)}] + 122.3617$$
$$\mathcal{EV} = 2.5058[\mathrm{ABC(G)}] + 33.8211$$
$$\mathcal{FP} = 12.5447[\mathrm{ABC(G)}] + 29.685$$
$$\mathcal{IR} = 0.005819[\mathrm{ABC(G)}] + 1.4569$$

Quadratic regression

$$\mathcal{BP} = -1.0740[\mathrm{ABC(G)}]^2 + 57.5397[\mathrm{ABC(G)}] - 151.3737$$
$$\mathcal{EV} = -0.1348[\mathrm{ABC(G)}]^2 + 7.1075[\mathrm{ABC(G)}] - 0.5269$$
$$\mathcal{FP} = -0.6626[\mathrm{ABC(G)}]^2 + 35.1703[\mathrm{ABC(G)}] - 139.1967$$
$$\mathcal{IR} = -0.0005[\mathrm{ABC(G)}]^2 + 0.0239[\mathrm{ABC(G)}] + 1.3218$$

Hyper Zagreb index

Linear regression

$$\mathcal{BP} = 0.5399[\mathrm{HM(G)}] + 194.4627$$
$$\mathcal{EV} = 0.06431[\mathrm{HM(G)}] + 42.7621$$
$$\mathcal{FP} = 0.3246[\mathrm{HM(G)}] + 73.0241$$
$$\mathcal{IR} = 0.0001532[\mathrm{HM(G)}] + 1.4756$$

Quadratic regression

$$\mathcal{BP} = -0.0007[\mathrm{HM(G)}]^2 + 1.2694[\mathrm{HM(G)}] + 41.0841$$
$$\mathcal{EV} = -0.0001[\mathrm{HM(G)}]^2 + 0.1575[\mathrm{HM(G)}] + 23.17$$
$$\mathcal{FP} = -0.0004[\mathrm{HM(G)}]^2 + 0.7752[\mathrm{HM(G)}] - 21.7045$$
$$\mathcal{IR} = 0.0000[\mathrm{HM(G)}]^2 + 0.0005[\mathrm{HM(G)}] + 1.3932$$

Geometric arithmetic index

Linear regression

$$\mathcal{BP} = 14.854[\mathrm{GA(G)}] + 138.9602$$
$$\mathcal{EV} = 1.7853[\mathrm{GA(G)}] + 35.7787$$
$$\mathcal{FP} = 8.9204[\mathrm{GA(G)}] + 39.8867$$
$$\mathcal{IR} = 0.00427[\mathrm{GA(G)}] + 1.4586$$

Quadratic regression

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	160.267	2.8813	-	0.8837	0.7809	49.9092	0.0000	Significant
$\mathcal{EV}$	16	38.4867	0.345	-	0.856	0.7327	38.3721	0.0000	Significant
$\mathcal{FP}$	16	52.6224	1.7309	-	0.8818	0.7775	48.9319	0.0000	Significant
$\mathcal{IR}$	16	1.4663	0.0008141	-	0.6707	0.4498	11.4454	0.0045	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−71.9402	7.785	−0.0220	0.9359	0.876	45.9274	0.0000	Significant
$\mathcal{EV}$	16	8.9052	0.9697	−0.0028	0.9131	0.8337	32.5761	0.0000	Significant
$\mathcal{FP}$	16	−89.8173	4.7389	−0.0135	0.9361	0.8762	46.0228	0.0000	Significant
$\mathcal{IR}$	16	1.3473	0.0033	0.0000	0.7937	0.63	11.0656	0.0016	Significant

Table 3. The QSPR model of $M_1(G)$ utilized statistical parameters.

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	195.8964	2.2579	-	0.867	0.7516	42.368	0.0000	Significant
$\mathcal{EV}$	16	42.891	0.2693	-	0.8364	0.6995	32.5964	0.0000	Significant
$\mathcal{FP}$	16	74.1823	1.3551	-	0.8643	0.747	41.3373	0.0000	Significant
$\mathcal{IR}$	16	1.4752	0.0006473	-	0.6676	0.4457	11.2584	0.0047	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−4.708	6.0844	−0.0150	0.9236	0.853	37.7237	0.0000	Significant
$\mathcal{EV}$	16	16.9859	0.7634	−0.0019	0.9001	0.8102	27.7447	0.0000	Significant
$\mathcal{FP}$	16	−48.0778	3.6873	−0.0091	0.9224	0.8509	37.0974	0.0000	Significant
$\mathcal{IR}$	16	1.3698	0.0027	0.0000	0.8049	0.6479	11.9593	0.0011	Significant

Table 4. The QSPR model of $M_2(G)$ utilized statistical parameters.

$$\mathcal{BP} = -0.5762[\mathrm{GA(G)}]^2 + 41.393[\mathrm{GA(G)}] - 125.5436$$
$$\mathcal{EV} = -0.0718[\mathrm{GA(G)}]^2 + 5.0924[\mathrm{GA(G)}] + 2.8184$$
$$\mathcal{FP} = -0.3528[\mathrm{GA(G)}]^2 + 25.1725[\mathrm{GA(G)}] - 122.0911$$
$$\mathcal{IR} = -0.0003[\mathrm{GA(G)}]^2 + 0.0174[\mathrm{GA(G)}] + 1.3278$$

Computed statistical parameters

Different parameters in a regression model have different purposes. The number of items (population) in a sample is represented by the quantity N. The constant and coefficient of topological index are represented by A, B, and C, respectively. The correlation coefficient between the predicted and actual values of the physicochemical properties is represented by r. The r values can indicate a direct relationship (positive value) or an inverse relationship (negative value). The r^2 provides an assessment of the relationship between independent variables changes and dependent variables. The regression model with the highest r^2 value is considered highly efficient. When the F value in any test is greater than 2.5, it is considered significant. The significance of the obtained data is indicated by the value of p. If the value of p$\leq$ 0.05, than the result is significant, otherwise insignificant. The regression model Tables 3-11 included the coefficients, the correlation coefficients, square of the correlation coefficients (r^2), F-ratio test, p values, and significance level.

Implementation of the ARASS (Additive Ratio Assessment) method

The additive ratio assessment method simplifies complex decision-making by selecting the best alternative based on a relative indicator, or utility degree. This indicator shows the difference between alternatives and the ideal solution while eliminating the influence of varying measurement units. It is a compensatory method in which both beneficial and non-beneficial attributes are considered to achieve a feasible solution. The advantage of this type of multi-attribute group decision-making method is that it requires minimal computing time, is easy to use, and maintains the independence of attributes. The steps involved in evaluating the alternatives are as follows:

Step 1: Decision-making matrix. The first step is establishing decision-making matrix as shown in Table 12.

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	112.6942	34.9958	-	0.8905	0.793	53.6271	0.0000	Significant
$\mathcal{EV}$	16	32.6182	4.2065	-	0.8659	0.7498	41.9456	0.0000	Significant
$\mathcal{FP}$	16	24.0447	21.0229	-	0.8886	0.7895	52.5158	0.0000	Significant
$\mathcal{IR}$	16	1.4532	0.009857	-	0.6738	0.454	11.64	0.0042	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−209.1402	104.1444	−3.2839	0.9423	0.8879	51.5057	0.0000	Significant
$\mathcal{EV}$	16	−7.3365	12.7911	−0.4077	0.9195	0.8455	35.5797	0.0000	Significant
$\mathcal{FP}$	16	−173.4218	63.45	−2.0149	0.9424	0.8882	51.6158	0.0000	Significant
$\mathcal{IR}$	16	1.2977	0.0433	−0.0016	0.7836	0.614	10.3415	0.0021	Significant

Table 5. The QSPR model of H(G) utilized statistical parameters.

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	183.8097	1.0558	-	0.8692	0.7555	43.2551	0.0000	Significant
$\mathcal{EV}$	16	41.4652	0.1259	-	0.8382	0.7025	33.0616	0.0000	Significant
$\mathcal{FP}$	16	66.7236	0.6344	-	0.8675	0.7525	42.5736	0.0000	Significant
$\mathcal{IR}$	16	1.4751	0.000291	-	0.6435	0.4141	9.8958	0.0072	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−26.5146	2.8319	−0.0031	0.9268	0.8589	39.5707	0.0000	Significant
$\mathcal{EV}$	16	14.1782	0.3563	−0.0004	0.9035	0.8164	28.9119	0.0000	Significant
$\mathcal{FP}$	16	−62.3027	1.724	−0.0019	0.9273	0.8599	39.9054	0.0000	Significant
$\mathcal{IR}$	16	1.3653	0.0012	0.0000	0.7858	0.6175	10.494	0.0019	Significant

Table 6. The QSPR model of F(G) utilized statistical parameters.

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
	16	168.7892	11.9335	-	0.8815	0.7771	48.816	0.0000	Significant
	16	39.4728	1.4302	-	0.8547	0.7304	37.9346	0.0000	Significant
	16	57.8769	7.1637	-	0.879	0.7726	47.576	0.0000	Significant
	16	1.4665	0.003456	-	0.6857	0.4702	12.4233	0.0034	Significant
Quadratic regression model									
	16	−6.5686	32.2857	−0.3874	0.9334	0.8713	44.0185	0.0000	Significant
	16	10.967	4.0046	−0.0490	0.9105	0.8291	31.527	0.0000	Significant
	16	−79.7183	19.59	−0.2365	0.9325	0.8695	43.3209	0.0000	Significant
	16	1.3514	0.0139	−0.0002	0.8047	0.6475	11.9401	0.0011	Significant

Table 7. The QSPR model of ISI(G) utilized statistical parameters.

$$X = \begin{bmatrix} X_{o1} & \cdots & X_{oj} & \cdots & X_{0n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ X_{i1} & \cdots & X_{ij} & \cdots & X_{in} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ X_{m1} & \cdots & X_{mj} & \cdots & X_{mn} \end{bmatrix}$$

Step 2: Identify the optimal performance rating for each attribute. The next step is to identify the best performance evaluation for each attribute. When there are no preferences among decision-makers, the following formula is used to determine the ideal performance ratings:

$$x_{0j} = \max_i x_{ij}, \text{if} \max_i x_{ij} \text{is preferable;} \quad (1)$$

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	188.9077	1.5949	-	0.8617	0.7425	40.3752	0.0000	Significant
$\mathcal{EV}$	16	41.9405	0.1908	-	0.8341	0.6957	32.0045	0.0000	Significant
$\mathcal{FP}$	16	70.2513	0.9558	-	0.8578	0.7358	38.9833	0.0000	Significant
$\mathcal{IR}$	16	1.4701	0.0004742	-	0.6882	0.4736	12.5948	0.0032	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−37.8644	4.5234	−0.0079	0.9156	0.8383	33.6856	0.0000	Significant
$\mathcal{EV}$	16	13.214	0.5618	−0.0010	0.8923	0.7962	25.3936	0.0000	Significant
$\mathcal{FP}$	16	−66.4361	2.7209	−0.0047	0.9120	0.8317	32.1246	0.0000	Significant
$\mathcal{IR}$	16	1.3522	0.002	0.0000	0.8125	0.6602	12.627	0.0009	Significant

Table 8. The QSPR model of AZI(G) utilized statistical parameters.

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	122.3617	20.8665	-	0.8959	0.8026	56.9323	0.0000	Significant
$\mathcal{EV}$	16	33.8211	2.5058	-	0.8703	0.7575	43.7204	0.0000	Significant
$\mathcal{FP}$	16	29.685	12.5447	-	0.8946	0.8004	56.1255	0.0000	Significant
$\mathcal{IR}$	16	1.4569	0.005819	-	0.6711	0.4504	11.4732	0.0044	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−151.3737	57.5397	−1.0740	0.9447	0.8925	53.9761	0.0000	Significant
$\mathcal{EV}$	16	−0.5269	7.1075	−0.1348	0.9220	0.8501	36.8534	0.0000	Significant
$\mathcal{FP}$	16	−139.1967	35.1703	−0.6626	0.9459	0.8948	55.2621	0.0000	Significant
$\mathcal{IR}$	16	1.3218	0.0239	−0.0005	0.7801	0.6085	10.1048	0.0023	Significant

Table 9. The QSPR model of ABC(G) utilized statistical parameters.

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	194.4627	0.5399	-	0.8831	0.7799	49.5966	0.0000	Significant
$\mathcal{EV}$	16	42.7621	0.06431	-	0.8509	0.7241	36.735	0.0000	Significant
$\mathcal{FP}$	16	73.0241	0.3246	-	0.8819	0.7777	48.9836	0.0000	Significant
$\mathcal{IR}$	16	1.4756	0.0001532	-	0.6731	0.4531	11.5974	0.0043	Significant
Quadratic regression model									
$\mathcal{BP}$	16	41.0841	1.2694	−0.0007	0.9321	0.8689	43.0827	0.0000	Significant
$\mathcal{EV}$	16	23.17	0.1575	−0.0001	0.9050	0.8191	29.438	0.0000	Significant
$\mathcal{FP}$	16	−21.7045	0.7752	−0.0004	0.9335	0.8714	44.056	0.0000	Significant
$\mathcal{IR}$	16	1.3932	0.0005	0.0000	0.7992	0.6387	11.4898	0.0013	Significant

Table 10. The QSPR model of HM(G) utilized statistical parameters.

$$x_{0j} = \min_i x_{ij}^*, \text{if} \max_i x_{ij}^* \text{is preferable.} \tag{2}$$

Step 3: Compute a normalized decision matrix. The attribute, whose preferable values are maximum are normalized as follows:

$$x_{ij} = \frac{x_{ij}}{\sum_{i=0}^{m} x_{ij}}. \tag{3}$$

The attribute, whose preferable values are minimum are normalized by applying two step procedure:

Properties	N	A	B	C	r	r^2	F(>2.5)	P($\leq$0.05)	Indicator
Linear regression model									
$\mathcal{BP}$	16	138.9602	14.854	-	0.8906	0.7931	53.6651	0.0000	Significant
$\mathcal{EV}$	16	35.7787	1.7853	-	0.8659	0.7497	41.9428	0.0000	Significant
$\mathcal{FP}$	16	39.8867	8.9204	-	0.8884	0.7892	52.4001	0.0000	Significant
$\mathcal{IR}$	16	1.4586	0.00427	-	0.6877	0.473	12.5634	0.0032	Significant
Quadratic regression model									
$\mathcal{BP}$	16	−125.5436	41.393	−0.5762	0.9408	0.8852	50.1069	0.0000	Significant
$\mathcal{EV}$	16	2.8184	5.0924	−0.0718	0.9183	0.8433	34.9822	0.0000	Significant
$\mathcal{FP}$	16	−122.0911	25.1725	−0.3528	0.9404	0.8844	49.7393	0.0000	Significant
$\mathcal{IR}$	16	1.3278	0.0174	−0.0003	0.7970	0.6353	11.3243	0.0014	Significant

Table 11. The QSPR model of GA(G) utilized statistical parameters.

Alternatives	M_1(G)	M_2(G)	H(G)	F(G)	ISI(G)	AZI(G)	ABC(G)	HM(G)	GA(G)
Optimization direction	max	max	max	max	max	max	max	min	min
Weights	0.20	0.12	0.231	0.19	0.08	0.04	0.13	0.002	0.007
Optimal values	186	223	16.1857	496	43.8476	311.8975	26.9839	62	6.6547
Acebutolol	110	120	10.7333	276	25.3667	171.0313	17.5460	516	22.9167
Ranolazine	154	175	14.4667	384	36.5667	255.6719	23.6508	734	32.0634
Metoprolol	80	85	8.2667	192	18.7176	130.125	13.0561	362	17.3590
Amlodipine	136	160	12.9667	346	32.4	240.625	20.6201	666	28.1511
Atenolol	86	91	8.5	212	19.75	128.875	13.9820	394	18.1281
Carvedilol	154	180	14.5333	378	37.5167	276.3281	23.2417	738	32.5462
Nitroglycerin	62	62	6.4	154	13.7	84.25	10.5558	278	13.0749
Nadolol	112	126	9.6333	304	25.2833	163.4080	16.9471	556	21.7590
Amyl nitrite	28	26	3.5667	62	6.3667	46.75	5.1685	62	6.6547
Nicorandil	66	70	6.9333	156	15.55	109.5156	10.8943	296	14.5173
Propranolol	92	103	8.8667	226	21.85	152.9063	14.3894	432	19.4364
Molsidomine	82	92	8.1	198	19.7167	142.7656	12.7969	382	17.6270
Nicardipine	176	205	16.0333	452	41.5167	290.75	26.6052	862	35.7423
Nifedipine	126	151	11.2333	334	29.5333	210.7656	18.6772	636	24.9605
Diltiazem	148	173	13.3667	380	35.0167	245.2188	22.2246	726	30.0103
Ivabradine	186	223	16.1857	496	43.8476	311.8975	26.9839	942	36.7746

Table 12. Decision matrix.

$$\overline{x_{ij}} = \frac{1}{x_{ij}^*}; \tag{4}$$

$$x_{ij} = \frac{x_{ij}}{\sum_{i=0}^{m} x_{ij}}. \tag{5}$$

See Table 13

Step 4: Compute a weighted normalized decision matrix. The weighted normalized performance evaluation are determined as follows:

$$v_{ij} = x_{ij}.w_j. \tag{6}$$

where w_j is the weight (importance) of the j attribute and x_{ij} is the normalized rating of the j attribute as shown in Table 14.

Step 5: Compute the overall performance index for every alternative. The total of the weighted normalized performance evaluation can be used to determine the overall performance index for every alternative, as shown following.

Alternatives	$M_1(G)$	$M_2(G)$	H(G)	F(G)	IS(G)	AZI(G)	ABC(G)	HM(G)	GA(G)
Optimal values	0.0938	0.0985	0.0870	0.0983	0.0940	0.0953	0.0887	0.2581	0.1530
Acebutolol	0.0554	0.0530	0.0577	0.0547	0.0544	0.0523	0.0577	0.0323	0.0444
Ranolazine	0.0776	0.0773	0.0778	0.0761	0.0784	0.0781	0.0777	0.0161	0.0318
Metoprolol	0.0403	0.0375	0.0445	0.0380	0.0401	0.0398	0.0429	0.0484	0.0586
Amlodipine	0.0685	0.0706	0.0697	0.0686	0.0694	0.0735	0.0678	0.0323	0.0361
Atenolol	0.0433	0.0402	0.0457	0.0420	0.0423	0.0394	0.0459	0.0323	0.0562
Carvedilol	0.0776	0.0795	0.0781	0.0749	0.0804	0.0844	0.0764	0.0161	0.0312
Nitroglycerin	0.0313	0.0274	0.0344	0.0305	0.0294	0.0257	0.0347	0.0645	0.0779
Nadolol	0.0565	0.0556	0.0518	0.0602	0.0542	0.0499	0.0557	0.0323	0.0468
Amyl nitrite	0.0141	0.0115	0.0192	0.0123	0.0136	0.0143	0.0170	0.2581	0.1530
Nicorandil	0.0333	0.0309	0.0373	0.0309	0.0333	0.0335	0.0358	0.0484	0.0701
Propranolol	0.0464	0.0455	0.0477	0.0448	0.0468	0.0467	0.0473	0.0323	0.0523
Molsidomine	0.0413	0.0406	0.0436	0.0392	0.0423	0.0436	0.0421	0.0484	0.0577
Nicardipine	0.0887	0.0905	0.0862	0.0896	0.0890	0.0888	0.0874	0.0161	0.0285
Nifedipine	0.0635	0.0667	0.0604	0.0662	0.0633	0.0644	0.0614	0.0323	0.0408
Diltiazem	0.0746	0.0764	0.0719	0.0753	0.0751	0.0749	0.0730	0.0161	0.0339
Ivabradine	0.0938	0.0985	0.0870	0.0983	0.0940	0.0953	0.0887	0.0161	0.0277

Table 13. Normalized decision matrix.

Alternatives	$M_1(G)$	$M_2(G)$	H(G)	F(G)	ISI(G)	AZI(G)	ABC(G)	HM(G)	GA(G)
Optimal values	0.0188	0.0118	0.0201	0.0187	0.0075	0.0038	0.0115	0.0005	0.0011
Acebutolol	0.0111	0.0064	0.0133	0.0104	0.0044	0.0021	0.0075	0.0001	0.0003
Ranolazine	0.0155	0.0093	0.0180	0.0145	0.0063	0.0031	0.0101	0.0000	0.0002
Metoprolol	0.0081	0.0045	0.0103	0.0072	0.0032	0.0016	0.0056	0.0001	0.0004
Amlodipine	0.0137	0.0085	0.0161	0.0130	0.0056	0.0029	0.0088	0.0001	0.0003
Atenolol	0.0087	0.0048	0.0106	0.0080	0.0034	0.0016	0.0060	0.0001	0.0004
Carvedilol	0.0155	0.0095	0.0180	0.0142	0.0064	0.0034	0.0099	0.0000	0.0002
Nitroglycerin	0.0063	0.0033	0.0079	0.0058	0.0024	0.0010	0.0045	0.0001	0.0005
Nadolol	0.0113	0.0067	0.0120	0.0114	0.0043	0.0020	0.0072	0.0001	0.0003
Amyl nitrite	0.0028	0.0014	0.0044	0.0023	0.0011	0.0006	0.0022	0.0005	0.0011
Nicorandil	0.0067	0.0037	0.0086	0.0059	0.0027	0.0013	0.0047	0.0001	0.0005
Propranolol	0.0093	0.0055	0.0110	0.0085	0.0037	0.0019	0.0061	0.0001	0.0004
Molsidomine	0.0083	0.0049	0.0101	0.0074	0.0034	0.0017	0.0055	0.0001	0.0004
Nicardipine	0.0177	0.0109	0.0199	0.0170	0.0071	0.0036	0.0114	0.0000	0.0002
Nifedipine	0.0127	0.0080	0.0140	0.0126	0.0051	0.0026	0.0080	0.0001	0.0003
Diltiazem	0.0149	0.0092	0.0166	0.0143	0.0060	0.0030	0.0095	0.0000	0.0002
Ivabradine	0.0188	0.0118	0.0201	0.0187	0.0075	0.0038	0.0115	0.0000	0.0002

Table 14. Weighted normalized decision matrix.

$$S_i = \sum_{i=1}^{n} v_{ij}. \tag{7}$$

See Table 15.

Step 6: Determine the utility degree.

$$K_i = \frac{s_i}{s_0} \tag{8}$$

where s_i and s_0 are the optimality attributes values as shown in Table 15.

Alternatives	S_i	K_i	ARASS ranking
Optimal values	0.0938	1.0000	
Acebutolol	0.0556	0.5928	8
Ranolazine	0.0770	0.8209	4
Metoprolol	0.0410	0.4371	13
Amlodipine	0.0690	0.7356	6
Atenolol	0.0436	0.4648	11
Carvedilol	0.0771	0.8220	3
Nitroglycerin	0.0318	0.3390	15
Nadolol	0.0553	0.5896	9
Amyl nitrite	0.0164	0.1748	16
Nicorandil	0.0342	0.3646	14
Propranolol	0.0465	0.4957	10
Molsidomine	0.0418	0.4456	12
Nicardipine	0.0878	0.9360	2
Nifedipine	0.0634	0.6759	7
Diltiazem	0.0737	0.7857	5
Ivabradine	0.0924	0.9851	1

Table 15. Optimality function, utility degree and ranking.

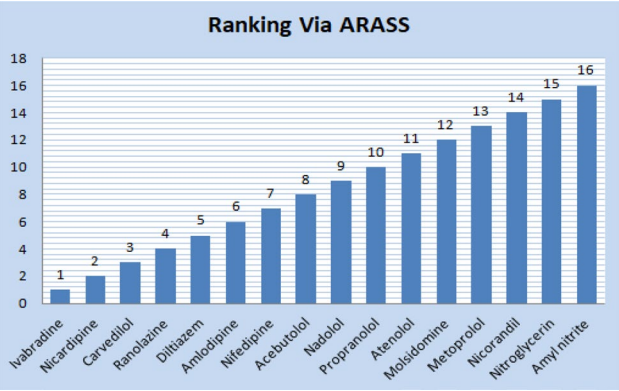


Fig. 2. Ranking of angina treatment medications via ARASS.

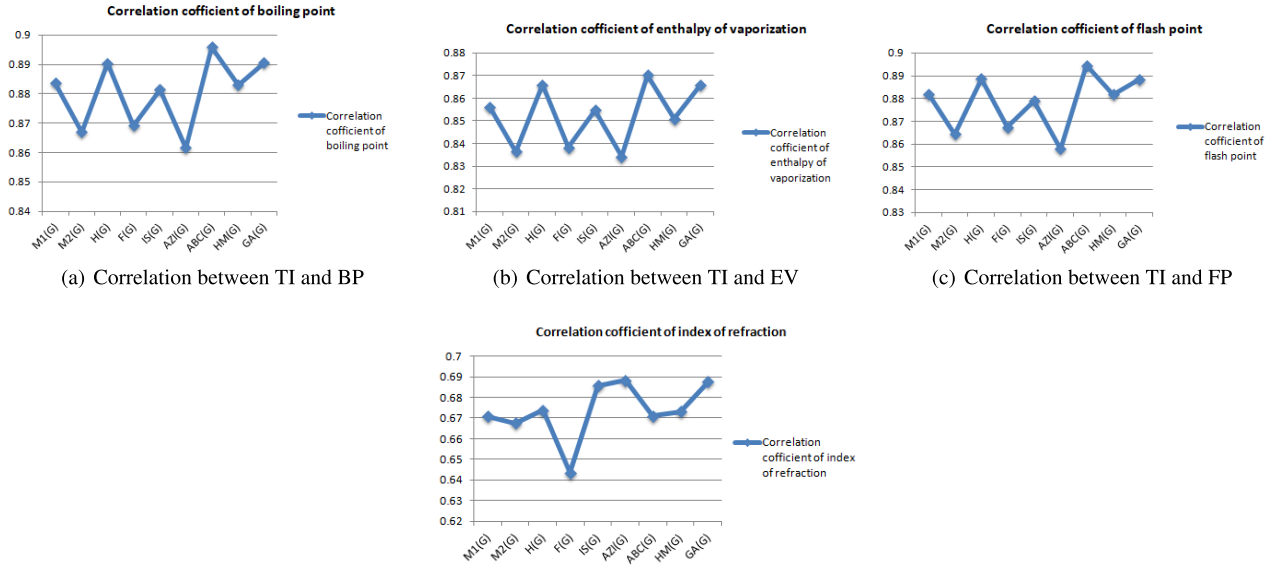
Step 7: Rank the alternatives and select the most effective one. After calculating K_i, the alternatives are ranked accordingly. For the given attribute, the alternative with the highest K_i' value is considered the best compromise solution and is ranked first, with the remaining alternatives ranked in descending order as shown in Table 15 and graphically shown in Fig. 2.

Graphical analysis of correlation coefficients

The correlation coefficient is a crucial measure because it indicates how well the theoretical models align with actual experimental data. This information can be valuable for chemists and pharmacists in developing effective treatments, including medications for angina. The P-value indicates the significance of the correlation coefficients. For results to be considered statistically significant, the P-value must be less than or equal to 0.05, and the correlation coefficients should lie within the range of −1 to 1. Values of the correlation coefficient for linear and quadratic regression models are shown in Table 16. Various types of graphs can be used to represent the data, including bar charts, line graphs, area graphs, curved graphs, scatter plots, pie charts, pictographs, column charts, and bubble charts. Fig. 3 and 4 show the relationship between properties and topological indices using curved graphs. The x-axis displays the names of the nine topological indices, while the y-axis shows the corresponding correlation values. Boiling point, enthalpy of vaporization, flash point, and index of refraction are physical properties of substances that often exhibit strong correlations with one another. All of the graphs have a positive x-axis because the topological indices (predicted values) and the properties (experimental values) are positively correlated. Ultimately, we find that the correlation coefficients and topological indices are significant.

Values of linear regression model				Values of quadratic regression model				
Topological indices	$\mathcal{BP}$	$\mathcal{EV}$	$\mathcal{FP}$	$\mathcal{IR}$	$\mathcal{BP}$	$\mathcal{EV}$	$\mathcal{FP}$	$\mathcal{IR}$
$M_1(G)$	0.8837	0.856	0.8818	0.6707	0.9359	0.9131	0.9361	0.7937
$M_2(G)$	0.867	0.8364	0.8643	0.6676	0.9236	0.9001	0.9224	0.8049
H(G)	0.8905	0.8659	0.8886	0.6738	0.9423	0.9195	0.9424	0.7836
F(G)	0.8692	0.8382	0.8675	0.6435	0.9268	0.9035	0.9273	0.7858
ISI(G)	0.8815	0.8547	0.879	0.6857	0.9334	0.9105	0.9325	0.8047
AZI(G)	0.8617	0.8341	0.8578	0.6882	0.9156	0.8923	0.9120	0.8125
ABC(G)	0.8959	0.8703	0.8946	0.6711	0.9447	0.9220	0.9459	0.7800
HM(G)	0.8831	0.8509	0.8819	0.6731	0.9321	0.9050	0.9335	0.7992
GA(G)	0.8906	0.8659	0.8884	0.6877	0.9408	0.9183	0.9404	0.7970

Table 16. Correlation coefficient of linear and quadratic regression models.



(a) Correlation between TI and BP (b) Correlation between TI and EV (c) Correlation between TI and FP

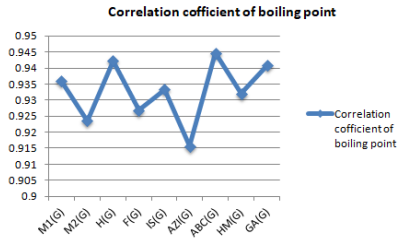
(d) Correlation between TI and IR

Fig. 3. Graphs of the correlation coefficient of the linear regression model.

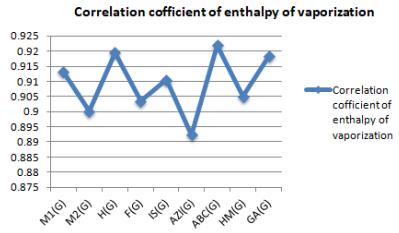
Applications of multi-attribute group decision-making

Multi-attribute group decision-making is a field within decision science that focuses on decision-making processes where a group of decision-makers evaluates multiple attributes. Multi-attribute group decision-making is widely applied across various fields because it effectively manages complex decision problems that involve multiple attributes and the input of various experts. Here are several key applications of multi-attribute group decision-making:

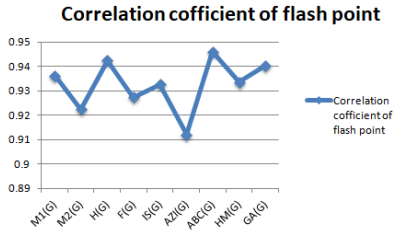
- In drug formulation, multi-attribute group decision-making techniques can be used to balance factors like drug stability, release rate, and patient compliance. This helps in designing formulations that meet both scientific and practical requirements. Multi-attribute group decision-making can assist in evaluating potential drug targets by assessing various attributes such as biological relevance, drug ability, and potential for off-target effects. This allows researchers to prioritize targets that are most promising for drug development. Multi-attribute group decision-making methods can help rank compounds based on multiple factors like biological activity, toxicity, and pharmacokinetics. This helps in selecting the most promising leads for further development.
- In transportation networks, communication networks, or supply chain logistics, multi-attribute group decision-making can be used to select the optimal path based on multiple criteria like distance, cost, time, and reliability. For designing transportation systems, such as road networks or public transit systems, multi-attribute group decision-making helps in selecting routes and connections by weighing factors like travel time, distance, cost, and safety. In designing communication networks (such as telecommunication or computer networks), multi-attribute group decision-making can be used to decide on the optimal network structure by considering multiple criteria like cost, bandwidth, latency, and reliability. Suppliers and manufacturers form



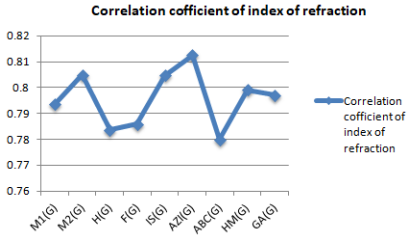
(a) Correlation between TI and BP



(b) Correlation between TI and EV



(c) Correlation between TI and FP



(d) Correlation between TI and IR

Fig. 4. Graphs of the correlation coefficient of the quadratic regression model.

Descriptor Set	Number of Descriptors	Computational Complexity	Interpretability	Predictive Accuracy
Our Degree-Based Topological Indices	∼9	Low	High	Comparable
RDKit	Hundreds	Medium	Medium	Good
Mordred	∼1800	High	Low–Medium	Good
alvaDesc	Several Hundred	Medium–High	Medium	Good

Table 17. Comparison of Molecular Descriptor Sets.

a network, and multi-attribute group decision-making can help in selecting the best suppliers by considering criteria such as cost, quality, delivery time, and reliability. The network of suppliers is analyzed using graph theory, and decision-makers evaluate potential suppliers to optimize the supply chain. Decision-makers evaluate different paths (edges) and nodes (vertices) to determine the best route that satisfies all individuals.

- In data analysis, graphs can represent relationships between data points, and multi-attribute group decision-making can be applied to cluster these data points based on multiple attributes like similarity, distance, or connectivity. Decision-makers evaluate different clustering options to find the most meaningful grouping. In large networks, identifying communities or clusters is crucial for understanding network dynamics. Multi-attribute group decision-making helps in partitioning the network into clusters by considering criteria like modularity, density, and edge.
- In education, multi-attribute group decision-making techniques are used to rank universities or academic programs based on criteria like academic performance, research output, faculty quality, and student satisfaction. Educational institutions apply multi-attribute group decision-making to design curricula that balance theoretical knowledge, practical skills, and industry relevance.
- Governments and organizations use multi-attribute group decision-making to develop energy policies by considering criteria like sustainability, cost, energy security, and public acceptance. Multi-attribute group decision-making is applied in evaluating renewable energy projects (e.g., wind, solar) by assessing environmental impact, cost, and energy output.

Results and discussion

QSPR models provide an overview of the relationship between chemical structures and biological activity, aiding in chemical analysis. QSPR models can predict the properties of novel molecular structures. This section discusses the relationship between physicochemical properties and chemical invariants as well as the results of linear and quadratic regression analyses. The approach developed in this study employs QSPR analysis to correlate the physical and chemical properties of angina drugs with specific topological descriptors. We analyzed the drugs using the assigned topological indices to achieve optimal outcomes. The goal is to identify the numerical values that exhibit a strong correlation.

In Table 17, we compare our degree-based topological indices with other commonly used molecular descriptor sets such as RDKit, Mordred, and alvaDesc. The table summarizes key aspects including the number of descriptors, computational complexity, interpretability, and predictive accuracy. Our approach uses only 9 descriptors, resulting in low computational complexity and high interpretability while achieving comparable

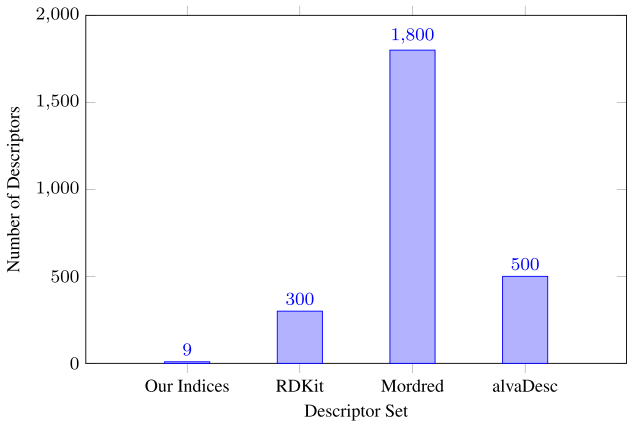


Fig. 5. Bar chart comparing the number of descriptors across different molecular descriptor sets.

predictive performance. In contrast, RDKit and alvaDesc offer approximately 300 and 500 descriptors respectively, with medium levels of complexity and interpretability, whereas Mordred provides around 1800 descriptors, which can lead to higher computational demands and reduced interpretability. Figure 5 graphically illustrates these differences by depicting the number of descriptors for each descriptor set, further emphasizing the streamlined and efficient nature of our method.

Conclusions

This research observed the properties of sixteen angina drugs, namely Acebutolol, Ranolazine, Metoprolol, Amlodipine, Atenolol, Carvedilol, Nitroglycerin, Nadolol, Amyl Nitrite, Nicorandil, Propranolol, Molsidomine, Nicardipine, Nifedipine, Diltiazem, and Ivabradine. One effective technique employed by scientists to reduce unnecessary laboratory costs is QSPR analysis, which uses topological descriptors for medications treating various diseases. A QSPR model was developed using linear and quadratic regression analysis to estimate properties such as boiling point, enthalpy of vaporization, flash point, and index of refraction. All topological indices demonstrated a strong correlation with these properties of the angina drugs. The prioritization of drugs can be viewed as a multi-attribute group decision-making challenge. The ARAS method is particularly flexible in addressing diverse decision-making scenarios, especially when decision-makers possess varying levels of expertise or when criteria weights may change. The method is designed to be robust, ensuring that the final rankings are consistent and reflect the collective preferences of the group. This approach facilitates the integration of both qualitative and quantitative criteria, making it particularly suitable for complex decision-making scenarios that involve multiple factors. To demonstrate the application of this effective multi-attribute group decision-making technique, sixteen angina medications were evaluated. The methodology relies heavily on thorough evaluations and has been successfully applied within the framework of topological indices. We identified ivabradine as the most suitable medication, closely aligning with the optimal solution. Future research in the field of angina treatment should focus on advancing personalized medicine, developing innovative pharmacological therapies, and leveraging regenerative medicine. The potential of regenerative medicine, including stem cell therapy and tissue engineering, should be a priority to restore damaged cardiac tissue. Integrating digital health technologies and artificial intelligence to improve real-time patient monitoring and personalized treatment plans will also be crucial in shaping the future of angina care.

Data availability

The datasets used or analysed during the current study available from the corresponding author on reasonable request

Received: 4 October 2024; Accepted: 13 May 2025
Published online: 11 August 2025

References

1. Balaban, A. T. Highly discriminating distance-based topological index. *Chemical Physics Letters* **89**(5), 399–404 (1982).
2. Gutman, I. Degree-based topological indices. *Croatica Chemica Acta* **86**(4), 351–361 (2013).
3. Mondal, S., Dey, A., De, N. & Pal, A. QSPR analysis of some novel neighbourhood degree-based topological descriptors. *Complex & Intelligent Systems* **7**, 977–996 (2021).
4. Arockiaraj, M. et al. Novel molecular hybrid geometric-harmonic-Zagreb degree based descriptors and their efficacy in QSPR studies of polycyclic aromatic hydrocarbons. *SAR and QSAR in Environmental Research* **34**(7), 569–589 (2023).
5. Paul, D., Arockiaraj, M., Jacob, K. & Clement, J. Multiplicative versus scalar multiplicative degree based descriptors in QSAR/QSPR studies and their comparative analysis in entropy measures. *The European Physical Journal Plus* **138**(4), 323 (2023).
6. Imani, A., Gunawan, Agung Santoso & A., & Suhartono, D.,. Interpretable machine learning in drug discovery: QSAR modeling of molecular properties for alzheimers disease using random forest. *International Journal of Computing and Digital Systems* **16**(1), 1–10 (2024).

7. Abubakar, M. S., Aremu, K. O., Aphane, M., Amusa, L. B. A QSPR analysis of physical properties of antituberculosis drugs using neighbourhood degree-based topological indices and support vector regression. Heliyon, 10(7),(2024). https://doi.org/10.1016/j.heliyon.2024.e28260.
8. Awan, N. U. H. et al. QSPR analysis for physiochemical properties of new potential antimalarial compounds involving topological indices. *International Journal of Quantum Chemistry* **124**(11), e27391 (2024).
9. Hasani, M. & Ghods, M. Topological indices and QSPR analysis of some chemical structures applied for the treatment of heart patients. *International Journal of Quantum Chemistry* **124**(1), e27234 (2024).
10. Kirana, B., Shanmukha, M. C., Usha, A. A QSPR analysis and curvilinear regression for various degree-based topological indices of quinolone antibiotics, (2024). https://doi.org/10.21203/rs.3.rs-3887676/v1.
11. Zhang, X., Bajwa, Z. S., Zaman, S., Munawar, S. & Li, D. The study of curve fitting models to analyze some degree-based topological indices of certain anti-cancer treatment. *Chemical Papers* **78**(2), 1055–1068 (2024).
12. Ravi, V. & Desikan, K. Curvilinear regression analysis of benzenoid hydrocarbons and computation of some reduced reverse degree based topological indices for hyaluronic acid-paclitaxel conjugates. *Scientific Reports* **13**(1), 3239 (2023).
13. Hui, Z. H., Naeem, M., Rauf, A. & Aslam, A. Estimating the physicochemical properties of antiemetics using degree-based topological descriptors. *Molecular Physics* **121**(5), e2189491 (2023).
14. Khan, A. R. et al. Fundamental aspects of skin cancer drugs via degree-based chemical bonding topological descriptors. *Molecules* **28**(9), 3684 (2023).
15. Zavadskas, E. K. & Turskis, Z. A new additive ratio assessment (ARAS) method in multicriteria decision-making. *Technological and economic development of economy* **16**(2), 159–172 (2010).
16. Junior, F., Darmawan, R. W. & Petriyansyah, S. Design of a decision support system for housing selection using the web-based additive ratio assessment (Aras) method. *Technology and Society Perspectives (TACIT)* **2**(2), 252–262 (2024).
17. Arshad, M. W. Implementation of entropy and additive ratio assessment methods in determining the best warehouse location. *Bulletin of Computer Science Research* **4**(4), 318–326 (2024).
18. Wahyudi, A. D. Analisis kepuasan terhadap pelayanan supplier menggunakan metode a new additive ratio assessment (ARAS). *Journal of Artificial Intelligence and Technology Information* **2**(1), 1–13 (2024).
19. Kirmani, S. A. K., Ali, P., Azam, F. & Alvi, P. A. On ve-degree and ev-degree topological properties of hyaluronic acid-anticancer drug conjugates with QSPR. *Journal of Chemistry* **2021**(1), 3860856 (2021).
20. Das, K. C. & Gutman, I. Some properties of the second Zagreb index. *MATCH Commun. Math. Comput. Chem* **52**(1), 3–1 (2004).
21. Gutman, I., Trinajstić, N. Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. Chemical physics letters, 17(4), 535-538. (1972).
22. Gutman, I., Ru Ić, B., Trinajstić, N., Wilcox Jr, C. F. Graph theory and molecular orbitals. XII. Acyclic polyenes. The journal of Chemical Physics, 62(9), 3399-3405, (1975).
23. Fajtlowicz, S. On conjectures of Graffiti. *In Annals of Discrete Mathematics* **38**, 113–118 (1988).
24. Furtula, B. & Gutman, I. A forgotten topological index. *Journal of Mathematical Chemistry* **53**(4), 1184–1190 (2015).
25. Vukičević, D., & Gašperov, M.,. Bond additive modeling 1. *Adriatic indices. Croatica Chemica Acta* **83**(3), 243–260 (2010).
26. Sedlar, J. & Stevanović, D., & Vasilyev, A.,. On the inverse sum indeg index. *Discrete Applied Mathematics* **184**, 202–212 (2015).
27. Estrada, E., Torres, L., Rodriguez, L., Gutman, I. An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, (1998).http://nopr.niscpr.res.in/handle/123456789/40308
28. Shirdel, G. H., Rezapour, H. & Sayadi, A. M. The hyper-Zagreb index of graph operations. *Iran. J. Math. Chem.* **4**(2), 213–220 (2013).
29. Vukicevic, D. & Furtula, B. Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *Journal of mathematical chemistry* **46**, 1369–1376 (2009).
30. Hakeem, A., Muhammad Katbar, N., Muhammad, F. & Ahmed, N. QSPR analysis of some important drugs used in heart attack treatment via degree-based topological indices and regression models. *Polycyclic Aromatic Compounds* **44**(8), 5237–5246. https://doi.org/10.1080/10406638.2023.2262697 (2024).
31. Hakeem, A., Ullah, A., Zaman, S., Hamed, Y. S. & Belay, M. B. Computational insights into flavonoid molecular structures and their QSPR modeling via degree based molecular descriptors. *Chemical Papers* **1–16**, https://doi.org/10.1007/s11696-024-03811-w (2024).
32. Hakeem, A. et al. Computational modeling of triangular?-graphyne using advanced topological methods. *International Journal of Modern Physics B* **2550133**, https://doi.org/10.1142/s0217979225501334 (2024).
33. Hakeem, A., Katbar, N. M., Shaikh, H., Tolasa, F. T. & Abro, O. A. Reverse degree-based topological indices study of molecular structure in triangular -graphyne and triangular -graphyne chain. *Frontiers in Physics* **12**, 1422098. https://doi.org/10.3389/fphy.2024.1422098 (2024).
34. Hakeem, A. et al. On the modeling and computation of molecular descriptors of a novel next-generation wonder material -graphyne and zig-zag Gamma graphyne nanoribbon. *Ain Shams Engineering Journal* **15**(10), 102868. https://doi.org/10.1016/j.asej.2024.102868 (2024).
35. Hakeem, A., Ullah, A. & Zaman, S. Computation of some important degree-based topological indices for?-graphyne and Zigzag graphyne nanoribbon. *Molecular Physics* **121**(14), e2211403. https://doi.org/10.1080/00268976.2023.2211403 (2023).
36. Rasheed, M. W. Curvilinear regression analysis and ranking of migraine treatment drugs using degree-based topological indices and the WASPAS method. *Computers in Biology and Medicine* **186**, 109657 (2025).
37. Mahboob, A., Amin, L., Rasheed, M. W. & Karamat, J. Multi-criteria decision making: Revealing Afinitor as the leading brain tumor drug Using CRITIC, CoCoSo, and MABAC methods combined with QSPR analysis via Banhatti indices. *Computers in Biology and Medicine* **188**, 109820 (2025).
38. Rasheed, M. W., Mahboob, A. & Hanif, I. Uses of degree-based topological indices in QSPR analysis of alkaloids with poisonous and healthful nature. *Frontiers in Physics* **12**, 1381887 (2024).

Funding

This research received no funding

Declarations

Competing interests

Authors have no conflict of interest.

Additional information

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