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Research article

Implementation of multi-criteria decision making for the ranking of drugs used to treat bone-cancer

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Abstract: The concept of "topological index" refers to a numerical value determined by the structure of a chemical network. It serves to determine the physicochemical and biological properties of diverse medications, offering a more precise depiction of the theoretical properties of organic materials, this is achieved through the utilization of degree-based topological indices. Because of the development of resistance to existing treatments and the unpleasant side effects associated with some current drugs, the hunt for new drugs remains a priority. In drug discovery, QSPR approaches are widely used to predict, from a chemical structure, the biological activity of potential novel drugs. Researchers can prioritize compounds for synthesis and optimize them to improve potency, preference, and other desired attributes by establishing a correlation between chemical features and biological activity. Rational drug design approaches incorporate research methodologies such as quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR), along with decision-making strategies. The goal of these strategies is to improve the biological activity and physicochemical qualities of existing leads. This research includes mathematical modeling of drug mechanisms utilizing multiple-criteria decision analysis and QSPR analysis. Furthermore, using decision-making techniques, I can determine the order of production for various drugs used to treat bone cancer based on their examination using QSPR analysis and topological indices.

Keywords: topological indices; QSPR; chemical graphs
Mathematics Subject Classification: 05C09, 05C12, 05C92, 92E10

1. Introduction

Bone is a highly active, continually changing kind of connective tissue that helps in mobility, mechanical support, and protecting important organs, and skeletal structure [5]. Although bone has a high functional stability and regeneration capacity, critical-sized defects caused by trauma, tumors, or infections can prohibit bone tissue from rebuilding on its own in some cases [1,15]. Primary bone cancer is a type of cancer that originates from cells within bones. Osteosarcoma (Malignant cells in this tumor form abnormal bone and have a propensity to spread), Ewing sarcoma (bone or soft tissue surrounding the bones developing malignancy), malignant fibrous histiocytoma (a specific kind of cancer that typically develops in soft tissue but can also develop in bone), and chondrosarcoma (collection of bone tumors formed comprised of cells that produce excessive amounts of cartilage) are a few examples of primary bone cancers. Pain and swelling in bones, weight loss, fever, reduction in movement flexibility, bones that are easily broken, and fatigue are the common symptoms of bone cancer. Cancer that has progressed from another region of the body to the bone is referred to as secondary bone cancer. Treatment of primary and secondary bone tumors is difficult because of difficulties with conventional therapies like medication resistance and disease recurrence [19]. Due to their complexity, heterogeneity, aggressive activity, and lack of considerable advancement in their treatment protocols throughout the years, bone tumors provide a medical challenge. Scientists and medical professionals have paid close attention to the therapy of bone cancer [6]. Making a decision is selecting a strategy from a set of feasible possibilities to solve a particular problem. In operations research, multiple-criteria decision analysis (MCDA) explicitly considers multiple, conflicting criteria. When difficult topics are adequately organized and numerous factors are openly considered, more knowledgeable and better conclusions are made. MCDM approaches are used in a variety of areas. For example, the superiority and inferiority ranking method (SIR method) is an MCDA that can handle real data and provides the system user with six possible preference structures. Multi-criteria decision-making (MCDM), a subfield of operations research, explicitly evaluates numerous conflicting criteria in decision-making in both ordinary life and in contexts like corporate, governmental, and pharmaceutical. In 1981, Ching-Lai Hwang and Yoon developed the Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS), also referred to as the multi-criteria decision analysis technique (MCDM) [14]. TOPSIS is based on the premise that the chosen option should be the closest to the positive ideal solution (PIS) and the furthest away from the negative ideal solution (NIS). The VIKOR technique is a multi-criteria decision-making (MCDM) or decision-analysis method. This method was created with the idea that, in situations when decisions must be made based on competing and incommensurable requirements, comp romise is appropriate for resolving conflicts. Because the decision-maker desires the outcome that is closest to the ideal, the alternatives are evaluated using all preset criteria. After assessing the alternatives, VIKOR selects the compromise option that is closest to the ideal. Po-Lung Yu brought VIKORE into MCDM in 1973 [36]. It has been recognized that important aspects affecting a drug molecule's quality include the enthalpic and entropic contributions to the binding affinity of drug candidates. This measurement offers a quick evaluation of the forces that promote ligand binding and is typically incorporated into the thermodynamic signature. The correlation between the melting point and dose of poorly soluble medicines and the fraction absorbed was given in [4]. To choose the best drug candidates, it will be crucial to have access to the thermodynamic signature early on in the drug discovery process [24].

2. Materials and methods

A graph is defined as a pair Ω = (V, Ɛ), where V is a set, whose elements are known as vertices and Ɛ is a set of paired vertices whose components are known as edges. A graph's order is determined by its vertex count, or |V|. The number of edges, |Ɛ|, in a graph determines its size. The number of vertices adjacent to vertex ω is used to represent the degree of a vertex ω, which is represented by the symbol d_ω. The terms "degree" and "valence" have some similarity in the field of chemistry. A molecular graph is a graph-theoretical depiction of the chemical compound's structural formula, where the atoms in the compound serve as the vertices and the chemical bonds that connect them as the edges. A topological index is a kind of molecular descriptor that is computed from the molecular graph of a chemical substance. A subfield of graph theory called chemical graph theory integrates mathematical modeling of chemicals. It places a focus on topological parameters that are closely related to the characteristics of molecular compounds. Quantitative structure-property/structure-activity relationship (QSPR/QSAR) modeling frequently uses topological indices to predict a molecule's physicochemical and bioactivity attributes [7]. Much research that aims to quantify and predict the physicochemical and biological properties of molecules continues to center on quantitative structure-property connections (QSPR), instead of expensive biological tests or studies, estimated descriptors of a certain physicochemical feature can be used to predict the reactions of interest for novel molecules [17]. QSPR models with linear regression between drug physicochemical parameters and several topological indices for Cardiac disease medications are given in [2]. S Nasir provided a QSPR analysis for Anti-cancer medications [20] whereas a QSPR analysis of drugs used to treat breast cancer was provided by S. Bokhary, [3]. The premise behind this study is that new drug structures may be identified, and their superiority can be assessed by examining them for various variables while keeping chemical indices in mind. This research includes mathematical modeling of pharmacological mechanisms. I can solve the obstacles of picking the most effective chemical compounds to employ in the development of new medications by applying QSPR analysis and the Vikor method. This integration is a novel approach that uses chemical indices produced from QSPR modeling in conjunction with operations research techniques to make informed medication prioritization decisions based on a variety of parameters including boiling point, complexity, and molar volume. In addition, the application of this integrated method extends beyond traditional chemical and pharmaceutical sectors into the world of biomedicine, where it gives a systematic framework for categorizing structures pertinent to biological and chemical sciences. The QSPR modeling is founded on nine topological indices, that are described in definitions 2.1–2.8.

Definition 2.1. ABC index [9] of Ω is given as:

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

Definition 2.2. Randic index [21] is given as:

$$RA(\Omega) = \sum_{uv\in E(\Omega)} \sqrt{\frac{1}{d_u d_v}}.$$

Definition 2.3. Sum connectivity index [37] of the graph Ω is given as:

$$S(\Omega) = \sum_{uv\in E(\Omega)} \sqrt{\frac{1}{d_u+d_v}}.$$

Definition 2.4. GA index [34] is defined as:

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

Definition 2.5. First and second Zagreb indices [12] are defined as:

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

$$M_2(\Omega) = \sum_{uv \in E(\Omega)} (d_u d_v).$$

Definition 2.6. Harmonic index [10] of a graph Ω is given as:

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

Definition 2.7. Hyper Zagreb index is defined [29] as:

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

Definition 2.8. Forgotten index denoted by F[11] can be defined as:

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

Shang, Y. provided Estrada index of dynamic random graphs In [28], readers are directed to refer [25,26,27] for interesting material regarding Topological indices.

3. Results

For medical and environmental chemistry, it is crucial to predict physical qualities like melting and boiling temperatures, enthalpy of vaporization, etc. To calculate a chemical compound's solubility, several physical factors are crucial. Researchers have conducted a significant amount of research on the accuracy of these physicochemical property predictions [33] as well as the connection between melting point and drug absorption [32]. Quantitative structure-property relationship (QSPR) modeling is a highly useful tool in cheminformatics. This strategy is founded on the notion that the variance in a chemical's physicochemical qualities is governed by its structural variation. Thus, in the lack of experimental data within a specific set, one can forecast the missing data using a proper mathematical model and designated molecular descriptors generated for each chemical in the set [30,31]. Rauf A. conducted a QSPR study on the medications used to treat breast cancer [22]. Rojas et al. used phase change contrast compounds with low boiling points [23] for in vivo molecular imaging. Using the Vikor technique, many researchers rank medications based on their physical features [13,16]. Considering the three physio-compound features of BP (boiling point), Molar volume, and Complexity, I intend to investigate the findings of the QSPR study into drugs used in the treatment of bone cancer.

Next, I looked at the significant outcomes of the QSPR modeling for bone cancer drugs. For this research, nine medications namely Doxorubicine, Ifosfamide, Gemcitabine, Etoposide, Methotrexate, Cisplatin, Zoledronic, Sunitinib, Regorafenib are being considered. I specifically analyze r (the

correlation coefficient) and SE (Standard Error) values for Boiling Point, Molar volume, and Complexity features concerning all chemical indices. In this case, the goal is to thoroughly examine every numerical component that represents a correlation value, are indicated in Table 1 correlation coefficient is closer to one and a smaller standard error suggests that the relevant chemical indices have a strong prediction potential concerning the desired qualities. This notion suggests that the desired results (r and SE) from QSPR are taken into consideration, Considering their significant roles in this in the account that both play a significant role in understanding how well-targeted chemical indices may predict the physicochemical features of targeted medicines. This notion suggests that the desired outcomes (r and SE) from QSPR are taken into consideration, recognizing their significant roles in determining the level to which particular chemical indices can accurately predict the physicochemical properties of individual drug. Furthermore, The standard error serves as both beneficial and non-beneficial criteria for each case presented in Table 2, corresponding to every drug and its chemical indices.

Table 1. Standard error and correlation coefficient between physical properties of bone cancer drugs.

Chemical indices	Boiling point		Complexity		Molar volume	
	Correlation coefficient	Standard error	Correlation coefficient	Standard error	Correlation coefficient	Standard Error
ABC(Ω)	0.633	155.0455	0.987	48.471	0.920	40.668
RA(Ω)	0.600	160.136	0.981	59.125	0.940	35.448
M_1(Ω)	0.645	152.973	0.992	37.777	0.901	45.059
M_2(Ω)	0.648	152.440	0.991	40.255	0.881	49.200
HM(Ω)	0.668	148.924	0.992	38.260	0.870	51.247
H(Ω)	0.584	162.593	0.977	64.742	0.946	33.636
S(Ω)	0.602	159.862	0.982	56.941	0.936	36.552
F(Ω)	0.686	145.609	0.991	41.127	0.857	53.437
GA(Ω)	0.605	159.446	0.984	53.979	0.930	38.056

Table 2. B (beneficial) and NB (non-beneficial) requirements for boiling point, complexity and Molar volume.

Topological indices	Boiling point	Complexity	Molar volume
ABC(**Ω**)	155.046	48.471	40.668
RA(**Ω**)	160.136	59.125	35.448
M_1(**Ω**)	152.973	37.777	45.059
M_2(**Ω**)	152.440	40.255	49.200
HM(**Ω**)	148.924	38.260	51.242
H(**Ω**)	162.593	64.742	33.636
S(**Ω**)	159.862	56.941	36.552
F(**Ω**)	145.609	41.127	53.437
GA(**Ω**)	159.446	53.979	38.056

3.1. Steps for weight calculation by CRITIC method

The CRITIC (Criteria Importance Through Intercriteria Correlation) method is a weighting technique employed to establish weights based on objective criteria. First presented in [8], it is centered on evaluating the levels of contrast and conflict in choice-making frameworks. To achieve this, the method utilizes correlation analysis to identify distinctions among criteria, as highlighted in [35]. In practice, the CRITIC method involves an evaluation of the decision matrix. It calculates the columns' standard deviation of the normalized criteria values and determines Coefficients of correlation to measure the contrast of the criterion for each pair of columns, as outlined by Madić and Radovanović [18].

The steps in the procedure for applying the CRITIC method are outlined in a study by Madić and Radovanović [18]. Initially, the method assumes the presence of a collection of m workable alternatives, denoted as Ai (where i = 1, 2, ..., p), whereas q Criteria for assessment, represented as C_j (where j = 1, 2, ..., q), under the specified problem context.

In first step a decision matrix, denoted as M, is created, depicting the performance of various alternatives in relation to different criteria.

$$M = \left[M_{ij}\right]_{p\times q}\begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1q} \\ m_{21} & m_{22} & \cdots & m_{2q} \\ \vdots & \vdots & \ddots & \\ m_{p1} & m_{p2} & \ldots & m_{pq} \end{bmatrix} \qquad \text{i = 1, 2, ..., p and j = 1, 2, ..., q,}$$

m_{ij} represents the conduct measurement for the ith Substitute regarding the jth criterion.

Second step involves normalizing the decision-matrix by applying The rule that follows.

$$m_{ij}^{*} = \frac{m_{ij}-\min\,(m_{ij})}{\max(m_{ij})-\min\,(m_{ij})} \qquad \text{i = 1, 2, ..., p and j = 1, 2, ..., q.}$$

The value represented by m_{ij}^{*} represents the normalized outcome of the ith alternative in relation to the jth criterion. In Step 3, when calculating the weights for criteria, the process takes into account both the criterion's standard deviation and correlation with other criteria. So, the weight assigned to the criterion (W_j), which is derived as follows:

$$W_j = \frac{C_j}{\sum_{j=1}^{q} C_j}.$$

Here, C_j represents the information content associated with the jth criterion and is determined as follows:

$$C_j = \sigma_j \sum_{j'=1}^{q}(1 - r_{jj'}).$$

Where σ_j represents the standard deviation of the jth criterion, and $r_{jj'}$ indicates the correlation coefficient between these two criteria.

Hower there are some complexities of CRITIC method such as pairwise correlation coefficients then normalizing the correlation matrix which become more complicated while handling large data. These complexities, increase the overall processing effort necessary to effectively apply the CRITIC technique. Nevertheless, the CRITIC approach is still computationally realistic for the majority of real-world scenarios and moderately sized decision-making problems.

3.2. Methodology for VIKOR and its implementation

The Bone cancer disease medications that are being examined as alternatives are evaluated in accordance with the predetermined criteria that I took into account within quantitative structure-property relationships (QSPR) are derived through observations in the case study in order to produce the best result for well-informed decision-making. Vikor ranks cancer disease medications and oversees the compromise treatment that is closest to the best. In 1973, Zeleny and Yu [36] introduced the compromise solution concept of MCDM.

Step 1. Identifying the optimal best $t_i^+$and optimal worst t_i^-values for $\{i = P_i, i = 1,\ldots,6\}$ for every criterion function that I took into account when predicting attributes.

t_i^+ ={maximum{ t_{ij}: j=1,2,...,j}, minimum { t_{ij}: j=1,2,...,j}:if the ith function proves to be favorable},

t_i^- ={minimum{ t_{ij}: j=1,2,...,j}, maximum { t_{ij}: j=1,2,...,j}:if the ith function proves to be favorable}.

Step 2. Calculating the values of the weighted normalized Chebyshev distance (R_j) and the weighted normalized Manhattan distance (S_j).with $j = \{1,\ldots,J\}$. The following equalities are available.

$$S_j = \sum_{j=1}^{m}[w_i \times \frac{(t_i^+ - t_{ij})}{(t_i^+ - t_i^-)}],$$

$$R_j = Max[w_i \times \frac{(t_i^+ - t_{ij})}{(t_i^+ - t_i^-)}].$$

Step 3. Determination of values $Q_j, j = 1,\ldots,J$, utilizing the subsequent equality

$$Q_j = [v \times \frac{(S_j - S^+)}{(S^- + S^+)}] + [(1 - v) \times \frac{(R_j - R^+)}{(R^- + R^+)}].$$

In contrast, the weight of each individual regret is (1-v). This tactic might be compromised with v 0.5.

Step 4. Ranking the possibilities by the values S, R, and Q from the lowest to the highest.

4. Discussion

In the investigation of BP, I acquired the stepwise calculations for steps 1 and 2 from Table 1(a) and Table 1(b) (available in suplimetry files), respectively, as well as the final computations for steps 3 and 4 in Table 3.

In the investigation of Complexity, I acquired the stepwise calculations for steps 1 and 2 from Table 2(a) and Table 2(b) (available in suplimetry files), respectively, as well as the final computations for steps 3 and 4 in Table 4.

In the investigation of Molar Volume, I acquired the stepwise calculations for steps 1 and 2 from Table 3(a) and Table 3(b) (available in suplimetry files), respectively, as well as the final computations for steps 3 and 4 in Table 5.

Table 3. Outputs for S_j, R_j, Q_j and rank for Boiling point (BP).

Drugs	S_j	R_j	Q_j	RANK
Doxorubicine	0.245	0.074	0.067	2
Ifosfamide	0.698	0.166	0.787	8
Gemcitabine	0.591	0.130	0.562	6
Etoposide	0.199	0.084	0.065	1
Methotrexate	0.427	0.073	0.213	4
Cisplatin	0.801	0.200	1.000	9
Zoledronic	0.611	0.132	0.586	7
Sunitinib	0.467	0.088	0.303	5
Regorafenib	0.415	0.067	0.179	3
S*, R*	0.199	0.067		
S_, R_	0.801	0.200		

Table 4. Outputs for S_j, R_j, Q_j and rank for complexity.

Drugs	S	R	Q	Rank
Doxorubicine	0.597	0.155	0.722	8
Ifosfamide	0.440	0.160	0.439	6
Gemcitabine	0.461	0.131	0.341	2
Etoposide	0.627	0.171	0.860	9
Methotrexate	0.559	0.106	0.409	4
Cisplatin	0.373	0.200	0.500	7
Zoledronic	0.440	0.142	0.352	3
Sunitinib	0.536	0.097	0.320	1
Regorafenib	0.557	0.107	0.410	5
S*, R*	0.373	0.097		
S_, R_	0.627	0.200		

Table 5. Outputs for S_j, R_j, Q_j and rank for Molar volume.

Drugs	S_j	R_j	Q_j	RANK
Doxorubicine	0.409	0.077	0.130	4
Ifosfamide	0.541	0.146	0.632	7
Gemcitabine	0.541	0.131	0.578	6
Etoposide	0.370	0.086	0.086	2
Methotrexate	0.414	0.062	0.085	1
Cisplatin	0.631	0.200	1.000	9
Zoledronic	0.573	0.147	0.700	8
Sunitinib	0.443	0.071	0.172	5
Regorafenib	0.421	0.062	0.100	3
S*, R*	0.370	0.062		
S_, R_	0.631	0.200		

The distribution of weights for boiling point, Complexity, and molar volume can be observed in Figures 1–3, respectively. Figure 4 gives a comparison between the ranks of all three physicochemical properties.

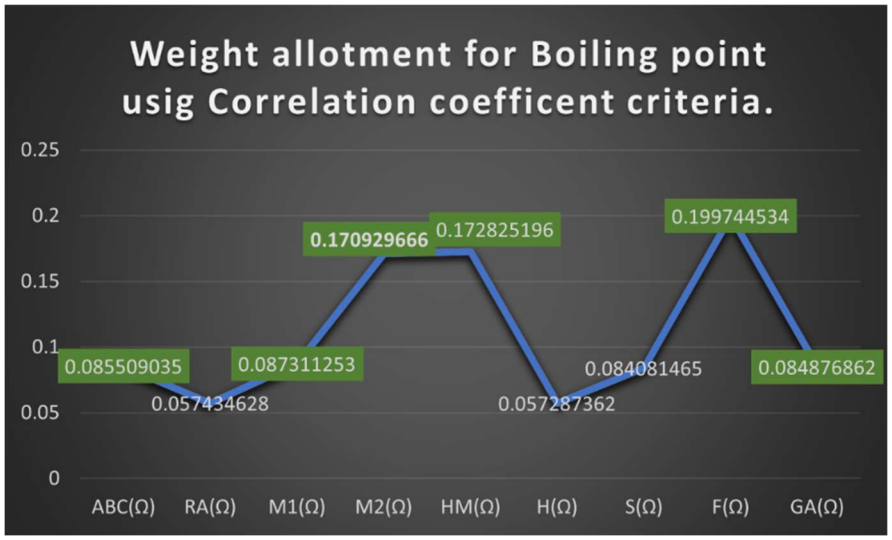

Figure1. Weight allocation for Boiling point with beneficial values are highlighted in green color.

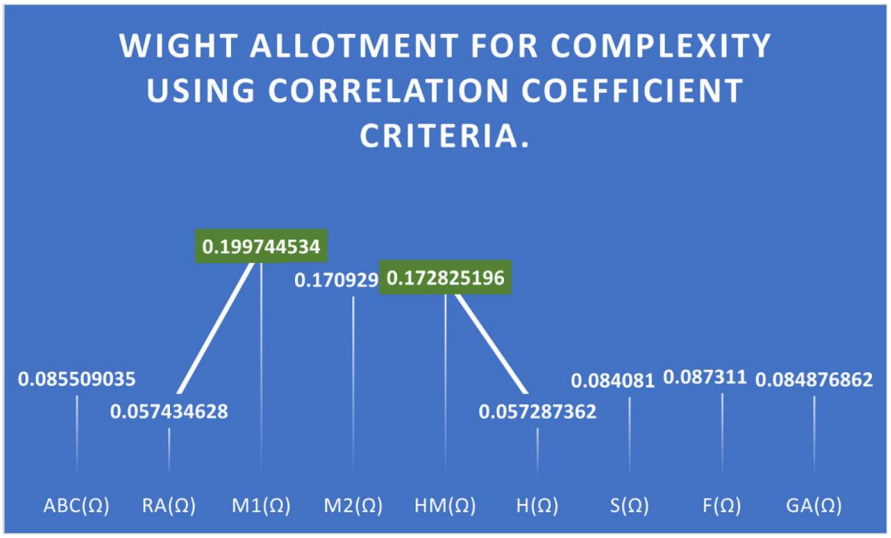

Figure 2. Weight allocation for Complexity with beneficial values are highlighted in green color.

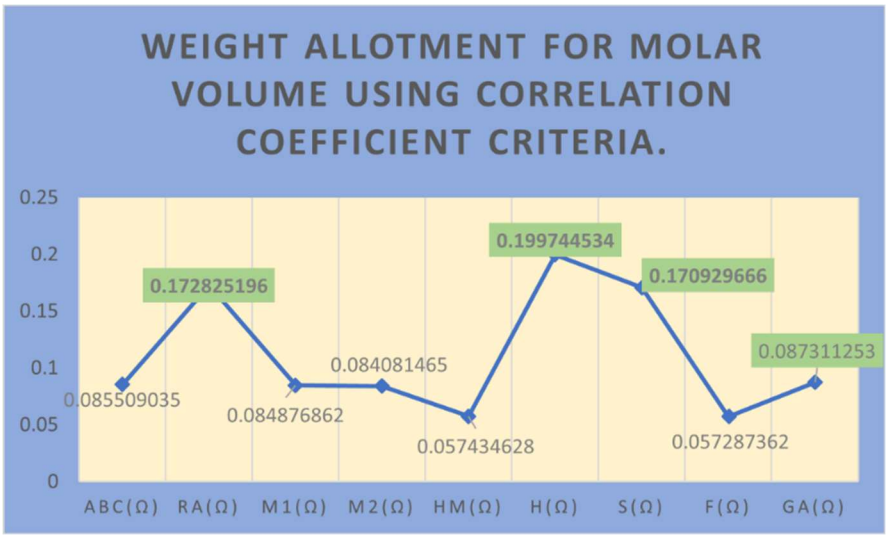

Figure 3. Weight allocation for Molar volume with beneficial values are highlighted in green color.

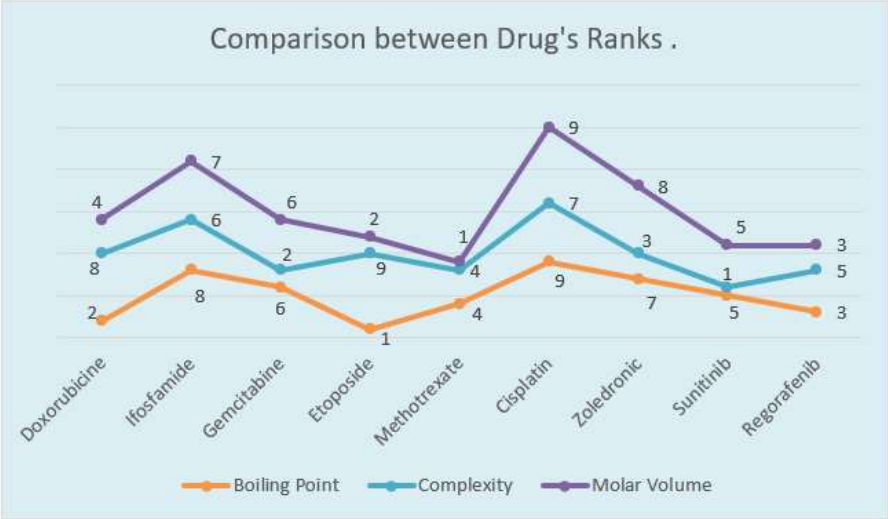

Figure 4. Comparison between the rank of BP, Complexity and Molar volume.

5. Conclusions

Nine Bone cancer disease medications (Doxorubicin, Ifosfamide, Gemcitabine, Etoposide, Methotrexate, Cisplatin, Zoledronic, Sunitinib, Regorafenib) have been addressed in the extremely pertinent VIKOR Multiple Criteria Decision Making (MCDM) methodology. The background setting for VIKOR has been observed under QSPR modeling by taking three properties, namely the boiling point, Complexity, and Molar volume into consideration. This ideology welcomes an entirely novel phase that will be useful for classifying any structure connected to biological and chemical sciences as well as biomedicine when a high call has been generated by chemical indices using QSPR and operation research techniques (MCDA) for the desired attributes and to see the impact on the rank ordering when addressing various structures and under specific circumstances by the evaluations obtained from QSPR By utilizing mathematical methods, this work will significantly advance the

chemical and pharmaceutical industries. However, there are a few limitations to the VIKOR approach for QSPR analysis, including data availability and quality, molecular complexity, model validation, and computational complexity. Overall, while VIKOR might serve as a useful tool for pharmacological QSPR analysis, given the limits of the VIKOR method, In the future researchers can employ alternative decision-making techniques to rank medications for usage in the healthcare industry.

Use of AI tools declaration

The author declares she has not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The author has no conflict of interest for this article.

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