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BOILING POINT MODELING OF EUGENOL COMPOUNDS AND ITS DERIVATIVES USING THE SOMBOR INDEX AND REDUCED SOMBOR INDEX APPROACHES

Alfian Putra Ardana[1], Syaftirridho Putri [2], Dia Lestari[3], I Gede Adithya Wisnu Wardhana[4*], Ni Komang Tri Dharmayani[5]

[1,2,4]*Departement Of Mathematics, Mataram University.*
[3,5]*Departement Of Chemistry, Mataram University.*
Email : [1]alfianputraardana93@gmail.com , [2] syaftirridho3@gmail.com ,
[3] dialestari668@gmail.com , [4*]adhitya.wardhana@unram.ac.id, [5] tri.dharmayani@unram.ac.id
[*]Coresponding Author

Abstract. Eugenol and its derivatives, phenylpropanoid compounds derived from plants like *Syzygium aromaticum*, exhibit significant biological activities, including antimicrobial, antifungal, anti-inflammatory, antioxidant, analgesic, and anticancer properties. These attributes make them valuable in drug development and medical applications. In mathematical chemistry, chemical topology graphs are used to determine the topological indices of molecules, which help predict physical and chemical properties. Here, atoms are represented as nodes and bonds as edges. This study explores the relationship between the Sombor index, the reduced Sombor index, and the boiling points of eugenol and its derivatives. The methodology includes literature review and computational analysis of the indices, followed by correlation analysis with the boiling points. The findings reveal that the Sombor index negatively correlates with the boiling point, accounting for 84.8% of the variation. This implies that an increase in the Sombor index results in a lower boiling point. Conversely, the reduced Sombor index demonstrates a positive correlation, influencing 36.1% of the boiling point variations, indicating that higher reduced Sombor indices correspond to higher boiling points. When combined, the Sombor and reduced Sombor indices explain 86.4% of the boiling point variance, highlighting their significance as predictive parameters. These results provide insights into the thermal properties of eugenol-based compounds and their potential applications in material and pharmaceutical sciences. By leveraging these indices, researchers can better predict and tailor the physical properties of eugenol derivatives for specific purposes.
Keywords: Eugenol, Chemical Topology Graph, Sombor Index, Reduced Sombor Index.

I. INTRODUCTION

In recent years, studies related to graph theory in describing algebraic structures have become an increasingly intensive focus of research. These research studies are concerned with the construction and properties of graphs that underlie the structure of mathematical groups[1]. Graph theory has many uses in mathematics, for example in algebraic structures, graphs are used to represent a group or ring. In chemistry, graphs can be used to solve molecular problems. Furthermore, graphs are closely related to topological indices. A topological index is a numerical value that reflects the structural properties and connectivity of a graph. These values are used to numerically represent chemical structures, as well as help predict various chemical properties, the physical structure of molecules, and their chemical reactions[2]. In the field of chemical topological graphs, graph theory is used to represent models of chemical molecules,

where atoms are treated as a set of corner points, and bonds between atoms form a set of edges in the graph[3].

One of the important topological indices in mathematical chemistry is the Sombor Index. This index was introduced by Ivan Gutman in 2021 and has a significant role in analyzing molecular structures. In graph theory, the Sombor Index is calculated based on the degree of connection between atoms in the molecule [4]. The Sombor Index is one of the topological parameters in quantum chemistry used to study molecular structures based on chemical graphs [5]. This index is useful for predicting physicochemical properties, molecular reactivity, and biological parameters in computational chemistry. The Sombor Index is known for considering the squared contribution of the vertex degree, which makes it different from other topological indices such as the Randić or Wiener Index [6]. The Reduced Sombor Index is a modification of the Sombor Index designed to provide a different perspective in molecular graph analysis. It calculates values based on the degree of vertices subtracted by one, making it more relevant for some chemical and molecular structure applications [7]. These two topological indices play an important role in predicting the physical properties of chemical molecular compounds by numerically calculating the molecular compounds by representing atoms as vertices and bonds between atoms as edges.

Eugenol is a natural phenolic compound found in various plants, especially in cloves (Syzygium aromaticum), bay leaves, cinnamon, and nutmeg. Eugenol has a distinctive aroma and various benefits that make it important in various fields [8]. Some derivatives of eugenol compounds are used in various specific fields such as the pharmaceutical field, perfume industry, cosmetics, food industry and agriculture [9]. The physical properties of eugenol compounds make it one of the important factors in its application, one of which is the boiling point. Usually, to find out the magnitude of the boiling point in chemical compounds, laboratory tests are carried out, but it can also be known by numerically calculating the compound using the calculation of the sombor index and the reduced sombor index [10].

Several previous studies have discussed the relationship between topological indices and the physicochemical properties of chemical compounds. These indices, such as the ABC Index and Zagreb index have been used to explain the relationship between molecular structure and properties such as boiling point and stability. For example, research conducted by Sabil, *et al.* (2025) found a relationship between boiling point and the stability of Calamenene basic framework compounds using the Zagreb index [11]. The results of this study showed that an increase in the Zagreb index value indicated that the boiling point of the compound tended to increase. However, in terms of stability, a higher Zagreb Index value actually indicates lower compound energy, which means that the compound has a higher level of stability. and research conducted by Pratiwi, et. al, where they successfully found a relationship between the ABC index and the physical properties of Prenylated Xanthone compounds [12]. The results of this study show that the addition of hydrophobic prenyl groups to xanthone derivatives contributes to increased molecular stability, increased biological activity, and decreased polarity and melting point.This article aims to model the effect of sombor index and reduced sombor index on eugenol compounds and their derivatives so that the results of the modeling can be used to determine the boiling point of eugenol compound derivatives without conducting laboratory tests.

II. MAIN RESULTS

This study aims to reveal the relationship pattern between molecular properties, such as boiling point with the Sombor index and the reduced Sombor index. Therefore, in this discussion, the results of the calculation of the Sombor index and the reduced Sombor index will be compared, and their relationship to the boiling point of eugenol compound derivatives will be analyzed. The following are the definitions of the Sombor index and the reduced Sombor index.

Definition 1. [11] *Suppose given a graph G with vertex set $V(G)$ and edge set $E(G)$. Then the summory index of G, denoted by $SO(G)$ is*

$$SO\ (G) = \sum_{(u,v)\in E(G)} \sqrt{d(u)^2 + d(v)^2}.$$

where $d(u)$ and $d(v)$ are the degrees or number of edges connected to vertices u and v.

Definition 2. [13] *Suppose a graph G with vertex set $V(G)$ and edge set $E(G)$ is given. Then the reduced Sombor index of G denoted by $SO_{red}(G)$ is*

$$SO_{red}(G) = \sum_{(u,v)\in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}.$$

where $d(u)$ and $d(v)$ are the degrees or number of edges connected to vertices u and v.

The Sombor index and the Reduced Sombor index are two related degree-based topological indices used to represent molecular structures in graph theory. The Sombor index measures the overall contribution of vertex degrees in a molecular graph, reflecting how each atom's connectivity affects molecular properties such as boiling point or molecular energy.

Meanwhile, the Reduced Sombor index modifies the classical form by reducing each vertex degree by one before calculation. This adjustment minimizes the dominance of vertices with high connectivity and provides a more balanced representation of molecular structures. In essence, the Sombor index emphasizes the actual connectivity of atoms, while the Reduced Sombor index focuses on the relative connectivity, offering a slightly different yet complementary perspective in molecular modeling.

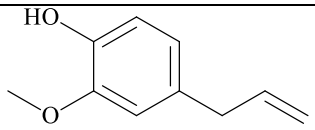
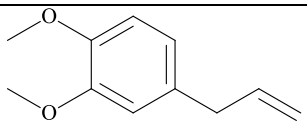
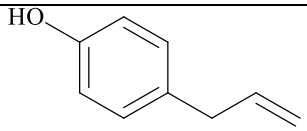
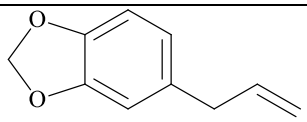
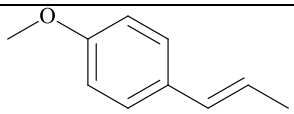
The definition above will be used in the calculation of the Chemical Topological Graph which is continued by analyzing the correlation between the values of the two indices with the boiling point of the eugenol compound derivatives. This analysis aims to understand the extent of the relationship between the structural parameters represented by the Sombor index and the reduced Sombor index with the physical properties of the compound, namely its boiling point. This section will present the results of research that discusses the boiling point model of five eugenol derivatives, with an approach using the Sombor index and the reduced Sombor index, as well as a comparison between the two models.

2.1 Compound Structure of Eugenol and its Derivatives

Eugenol and its derivatives are compounds of the phenylpropanoid pathway that have an aromatic ring-based structure (C6) with a three-carbon chain (C3), in which the hydroxyl (-OH) and methoxyl (-OCH_3) groups on the aromatic ring provide characteristic chemical properties and affect physical properties such as boiling point. These compounds are produced through the transformation of p-coumaryl-CoA which is a common precursor in the phenylpropanoid pathway through a series of specific enzymatic reactions producing compounds such as eugenol and its derivatives.

The following are the molecular structures and boiling points of 5 eugenol-derived compounds for which the Sombor index and reduced Sombor index will be calculated:

Table 2.1. 1 molecular image, boiling point, and compound name of eugenol derivatives

No.	Compound Name	Structure	Boiling Point (°C)
1.	Eugenol		254
2.	Methyl Eugenol		255
3.	4-Allylphenol		238
4.	Safrole		234
5.	Anethole		234

2.2 Modeling the Effect of Sombor Index on Eugenol Compound Derivatives

In this section we will discuss the calculation of the Sombor index of eugonol compound derivatives, the Sombor index on eugenol compound derivatives is calculated based on the groups in the chemical structure. Here is one of the calculation results of the eugenol compound:

$$SO\ (G) = \sum_{(u,v)\in E(G)} \sqrt{{d_u}^2 + {d_v}^2}$$

$$= \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{H\}}} \sqrt{d(u)^2+d(v)^2} + \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{C*\}}} \sqrt{d(u)^2+d(v)^2}$$
$$+ \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{C**\}}} \sqrt{d(u)^2+d(v)^2} + \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OH\}}} \sqrt{d(u)^2+d(v)^2}$$
$$+ \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OCH_3\}}} \sqrt{d(u)^2+d(v)^2}$$
$$= \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{H\}}} \sqrt{3^2+1^2} + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{C*\}}} \sqrt{3^2+3^2} + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{C**\}}} \sqrt{2^2+2^2}$$
$$+ \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OH\}}} \sqrt{3^2+1^2} + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OCH_3\}}} \sqrt{3^2+2^2}$$
$$= 5\sqrt{10} + 6\sqrt{18} + \sqrt{8} + \sqrt{10} + \sqrt{13}$$
$$= 50.8$$

In the modeling of eugenol and its derivatives, each molecule is represented as an undirected graph where atoms correspond to vertices and chemical bonds correspond to edges.

The terms $d(u)$ and $d(v)$ denote the degrees of the vertices u and v, respectively, which represent the number of bonds connected to each atom in the molecular structure [14]. For instance, a carbon atom (C) bonded to three other atoms has a degree of three, whereas a hydrogen atom (H) bonded to only one carbon atom has a degree of one [13].

The symbols C, H, $C*$, and $C**$ are used to distinguish different types of carbon atoms based on their bonding environments. For example:

- C represents a regular carbon atom in the main chain,
- $C*$ indicates a carbon atom attached to a functional group such as a hydroxyl or methoxy group,
- $C**$ refers to a carbon atom located in the aromatic ring with conjugated double bonds,
- H denotes a hydrogen atom connected to a carbon atom through a single bond.

Therefore, the vertex degree in the molecular graph reflects the structural connectivity of each atom in the eugenol compound. These degree values are then used in the computation of the Sombor and Reduced Sombor indices to evaluate the relationship between the molecular structure and the boiling point properties of the compounds [15].

For the calculation results of the Sombor index on other eugenol compound derivatives, see table 2.2.1

.

Below are the boiling point values and Sombor index of five eugenol derivatives:

Table 2. 2. 1 Boiling Point Value and Sombor Index of Eugenol Derivative Compounds

Compound	Boiling Point (°C)	Sombor Index
Eugenol	254	50.8
Methyl Eugenol	249	57.1
4- Allylphenol	238	58.9
Safrole	234	62.9
Anethole	234	66.6

Based on the boiling point and Sombor index in table 2.2.1, a linear regression analysis can be performed to determine the relationship pattern. The correlation between the boiling point and the Sombor index value of the eugenol compound derivative is relatively strong, the following are the results of the linear regression analysis.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.924[a]	.853	.804	4.06202

a. Predictors: (Constant), SO

Figure 2.2. 1 Model summary of the regression analysis between the Sombor index (SO) and the boiling points of eugenol compounds.

Based on Figure 2.2.1, the correlation coefficient (R) of 0.924 indicates a very strong and positive relationship between the Sombor index (SO) and the boiling points of eugenol compounds. The R Square (R^2) value of 0.853 suggests that approximately 85.3% of the variation in boiling point can be explained by variations in the Sombor index, while the remaining 14.7% is influenced by other factors not included in the model. The Adjusted R Square value of 0.804 shows that, after adjusting for the number of data points and predictor variables, the Sombor index still accounts for about 80.4% of the variation, confirming its strong explanatory power. Meanwhile, the Standard Error of the Estimate (4.06202) indicates the average deviation between the predicted and actual boiling point values. This relatively small error value compared to the overall data range implies that the regression model has a good level of predictive accuracy.

Overall, these results demonstrate that the Sombor index can serve as a significant topological descriptor for modeling the physicochemical properties of eugenol compounds, particularly their boiling points.

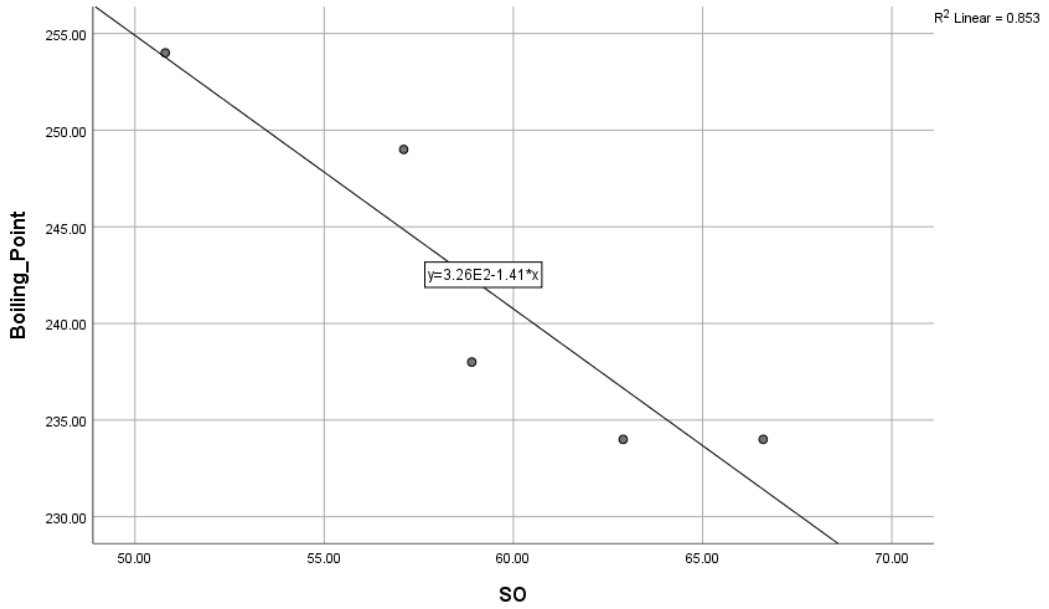


Figure 2.2. 2 Correlation Chart of Sombor Index to Boiling Point

Figure 2.2.2 shows the linear regression relationship between the Sombor index (SO) and the boiling points of eugenol compounds. The regression equation obtained is

$$Boiling\ Point\ (BP) = 3{,}26 + 1{,}41(SO)$$

with an R^2 value of 0.853. This result indicates a strong negative correlation between the Sombor index and the boiling point. The high R^2 value suggests that variations in the Sombor index can explain a large portion of the changes in boiling points among the eugenol compounds studied. The negative slope of the regression line implies that as the Sombor index increases, the boiling point tends to decrease.

Overall, the model demonstrates a good fit, meaning that the Sombor index serves as a reliable descriptor for predicting the boiling points of the examined compounds. However, further validation with a broader range of molecular structures is recommended to confirm the robustness of this correlation.

2.3 Modeling the effect of Reduced Sombor Index on 5 Eugenol derivatives

In this section will be discussed about the calculation of the reduced spear index of eugonol compound derivatives, the reduced spear index on eugenol derivatives is calculated based on the groups in the chemical structure. here is one of the calculation results of eugenol compounds:

$$SO_{red}\ (G) = \sum_{(u,v)\in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}$$

$$= \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{H\}}} \sqrt{(d(u)-1)^2+(d(v)-1)^2}$$
$$+ \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{C*\}}} \sqrt{(d(u)-1)^2+(d(v)-1)^2}$$
$$+ \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{C**\}}} \sqrt{(d(u)-1)^2+(d(v)-1)^2}$$
$$+ \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OH\}}} \sqrt{(d(u)-1)^2+(d(v)-1)^2}$$
$$+ \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OCH_3\}}} \sqrt{(d(u)-1)^2+(d(v)-1)^2}$$
$$= 23.30$$

Similar to sombor index, in the modeling of eugenol and its derivatives, each molecule is represented as an undirected graph where atoms correspond to vertices and chemical bonds correspond to edges.

The terms $d(u)$ and $d(v)$ denote the degrees of the vertices u and v, respectively, which represent the number of bonds connected to each atom in the molecular structure. the difference is that the degree-induced index at each node is reduced by one. For instance, a carbon atom (C) bonded to three other atoms has a degree of three, whereas a hydrogen atom (H) bonded to only one carbon atom has a degree of one.

For the calculation results of the reduced spear index on other eugenol compound derivatives, see Table 3.1.

The following is the boiling point value and reduced Sombor index on 5 Eugenol derivatives:

Compound	Boiling Point (℃) (BP)	Reduced Sombor Index (SO_{red})
Eugenol	254	23.30
Methyl Eugenol	249	24.54
4- Allylphenol	238	20.07
Safrole	234	25.37
Anethole	234	20.70

Based on the linear regression analysis, it was found that the correlation between the boiling point and the value of the reduced Sombor index is relatively weak, here are the results of the linear regression analysis.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.296[a]	.088	-.216	10.12061

a. Predictors: (Constant), SO_Red

Figure 2.3.1 Model summary of the regression analysis between the Sombor index (SO) and the boiling points of eugenol compounds.

Based on Figure 2.3.1, the correlation coefficient (R) of 0.296 indicates a weak positive relationship between the Reduced Sombor index (SO_{red}) and the boiling points of eugenol compounds. The R Square (R^2) value of 0.088 shows that only about 8.8% of the variation in boiling point can be explained by variations in the Reduced Sombor index, while the remaining 91.2% is influenced by other factors not included in the model. The Adjusted R Square value of -0.216 suggests that the model does not provide a good fit for the data, possibly due to the small sample size or the limited variation in the molecular structures analyzed. The relatively large Standard Error of the Estimate (10.12061) indicates that the predicted boiling points deviate considerably from the observed values, implying low predictive accuracy.

Overall, these results suggest that the Reduced Sombor index (SO_Red) has a weak correlation with the boiling points of eugenol compounds. Further studies involving a larger dataset and additional molecular descriptors are recommended to improve the accuracy and reliability of the regression model.

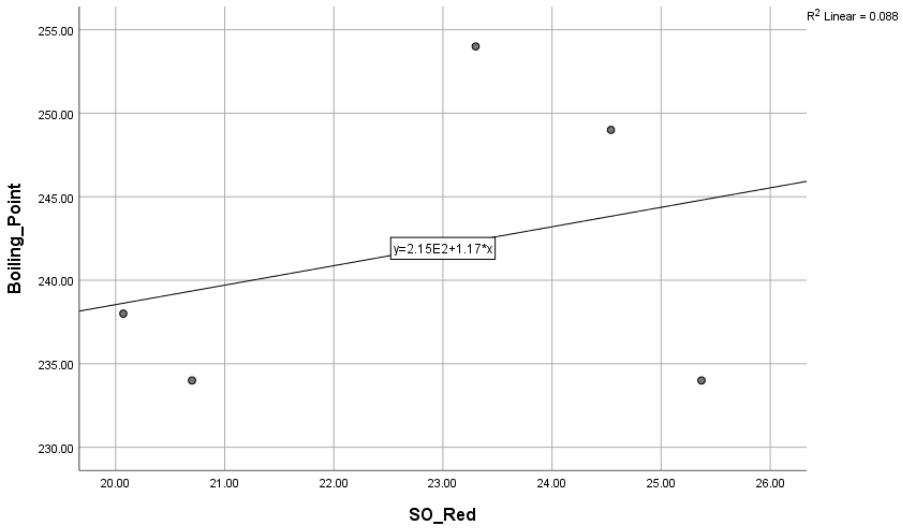


Figure 2.3.2 Correlation Chart of Reduced Sombor Index to Boiling Point

Figure 2.3.2 shows the linear regression relationship between the Reduced Sombor index (SO_{red}) and the boiling points of eugenol compounds. The regression equation obtained is.

$$Boiling\ Point\ (BP) = 2{,}15 + 1{,}17(SO_{red})$$

with an R^2 value of 0.088. This result indicates that the relationship between the Reduced Sombor index and the boiling point is weak, as reflected by the small R^2 value. The positive slope of the regression line suggests that, in general, an increase in the Reduced Sombor index corresponds to a slight increase in the boiling point. However, the data points are widely scattered around the regression line, showing that the model cannot accurately predict the boiling points of eugenol compounds based on the SO_{red} values alone.

The low coefficient of determination implies that the Reduced Sombor index contributes minimally to explaining the variation in boiling points. This may be due to the limited number of data points or the similarity in molecular structures among the compounds analyzed. Therefore, it is recommended that future research include more diverse compounds and a larger dataset to achieve a more reliable correlation.

2.4 Modeling the effect of Sombor index and Reduced Sombor Index on Eugenol derivatives

Based on the explanation in points 1 and 2 above, it is found that the results of the analysis using linear regression get the result that the Sombor index is more influential on the 5 turnan of eugenol compounds compared to the reduced Sombor index. The following are the results of regression analysis for both independent variables, namely Sombor index and reduced Sombor index to the boiling point:

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.927[a]	.860	.720	4.85890

a. Predictors: (Constant), SO, SO_Red

Figure 2.4.1 Correlation of Sombor Index and Reduced Sombor Index at Boiling Point

In Figure 2.4.1, it is found that the correlation that occurs between the boiling point when using both variables, namely the Sombor index and the reduced Sombor index, has a very strong correlation because the R value is 0.92,7 or 92,7%, meaning that the Sombor index and the reduced Sombor index have an influence on the boiling point. It's just that for the reduced Sombor index there is a weak correlation of 29,6% and the Sombor index has a relatively strong correlation of 92,4%.

The following is a table to determine the regression model of the boiling point by the Sombor index and the reduced Sombor index:

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients		
		B	Std. Error	Beta	t	Sig.
1	(Constant)	316.259	38.669		8.179	.015
	SO_Red	.333	1.072	.085	.311	.785
	SO	-1.385	.417	-.904	-3.319	.080

a. Dependent Variable: Boiling_Point

Figure 2.4.2 Estimation of the Relationship Pattern of Sombor Index and Sombor Index to Boiling Point

Figure 2.4.2 shows the coefficients of the multiple linear regression model between the boiling points of eugenol compounds and the predictors Sombor index (SO) and Reduced Sombor index SO_{red}. The regression equation obtained from the unstandardized coefficients is:

$$Boiling\ Point\ (BP) = 316.259 + 0.333(SO_{red}) - 1.385(SO).$$

The constant value of 316.259 represents the estimated boiling point of eugenol compounds when both the Sombor index (SO) and the Reduced Sombor index (SO_{red}) are equal to zero. The positive coefficient of SO_{red} (0.333) indicates that, when the Sombor index is held constant, an increase in the Reduced Sombor index tends to cause a slight increase in the boiling point. However, since the effect is small and statistically insignificant, SO_{red} contributes minimally to the model. Conversely, the coefficient of SO (-1.385) is negative, suggesting that as the Sombor index increases, the boiling point decreases. This implies that compounds with higher SO values generally have lower boiling points. Among the two descriptors, SO has a stronger influence on the boiling point, as indicated by its larger coefficient and higher statistical relevance.

In summary, the model shows that the boiling point of eugenol compounds is more strongly and inversely affected by the Sombor index (SO) than by the Reduced Sombor index (SO_{red}). This suggests that structural characteristics captured by the Sombor index play a more dominant role in determining the boiling behavior of these compounds.

III. CONCLUSIONS

In this study, the effect of Sombor index on the boiling point of eugenol compound derivatives is 85,3% which is negatively correlated, meaning that the higher the Sombor index, the boiling point decreases, and vice versa. The regression model to predict the boiling point using the Sombor index is $Boiling\ Point\ (BP) = 3{,}26 + 1{,}41(SO)$. The effect of the reduced Sombor index on the boiling point of eugenol compound derivatives has an effect of 0,088% which is positively correlated, meaning that the higher the reduced Sombor index, the boiling point increases, and vice versa. The effect of Sombor index and reduced Sombor index on the boiling point of eugenol compound derivatives is 86.0% which has a strong influence on the boiling point. The regression model to predict the boiling point using the Sombor index and the reduced Sombor index is $Boiling\ Point\ (BP) = 316.259 + 0.333(SO_{red}) - 1.385(SO)$. These are the results obtained in this study related to the effect of Sombor index and reduced Sombor index and its regression model on the boiling point of eugenol and its derivatives.

Further research may focus on expanding the dataset and incorporating additional molecular structures to improve the robustness of the predictive model and to validate the correlation between the Sombor-based indices and experimental boiling points.

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