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Application of Zagreb Index Models in Predicting the Physicochemical Properties of Unsaturated Fatty acids

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ABSTRACT

This paper develops models of the Zagreb index suitable for unsaturated fatty acids, which are crucial in performing metabolic functions in all living organisms. An algorithm-based methodology was brought into practice to optimize computation and data processing. Degree-based topological indices derived from the M-polynomial were computed using SPSS. Using linear regression analysis, the study proved that these indices are relevant to some physical properties of unsaturated fatty acids. The QSPR (Quantitative Structure-Property Relationship) models were developed to measure the efficiency of the models, making a correlation with four physical properties (LogP, Enthalpy, Molar Refractivity and Polarizability) and the indices. Right from the analyzed data, several multivariate linear regression models were built to find possible significant effects. It was concluded that the computed feature values adequately predict these physical properties' values, with the features' estimates showing great concentration on the observed values. Thus, the estimates regrettably relied on these values.

Keywords: Chemical graph theory, Unsaturated fatty acids, Zagreb index, Quantitative Structure-Activity Relationship, Quantitative Structure-Property Relationship.

INTRODUCTION

One of the critical areas of mathematics is graph theory, whose primary purpose is to study the relations, and the structures of graphs made of vertices (or nodes) and edges, representing the links between the elements in a set. Graph theory began in the 18th century in connection with the formulation and solution of mathematical problems and has now become a vital area of research with innumerable application areas in the sciences. Graph theory's relevance and significance are quite broad, particularly in the areas of chemistry, social sciences, and information technology[1,2,3].

Chemical Graph Theory (CGT) lies in the conjunction zone of graph theory and chemistry and allows a deep analysis of the atomic structure of chemical compounds[4]. In CGT, molecules are depicted as graphs whose vertices represent the atoms, and the edges represent the chemical bonds. This makes it possible for chemists to numerically study the chemical properties of chemical substances using mathematical graphs

and computer methods[5,6]. This directional growth of the scientific fields has been tremendous, and the alternative solutions generated in the growth of this science have stimulated the exploration of the structures of the molecules[7].

As one of the cornerstones of CGT, chemical indexes are mathematical tools that link molecular graphs of structures with associated properties. Such indices help interpret chemical properties from a graphical perspective[8]. Applying CGT to real-world chemical problems also emphasizes the revolutionary aspect of this approach. In the system that explains chemical structures using graphs, CGT provides more information about molecular architecture and reactivity and further relates the chemical behaviour of a substance to its structure. As integrated with chemistry, mathematics is an exciting and valuable tool for reasoning about the properties of chemical compounds.

Graph-based representations of chemical structures are essential in information retrieval, search algorithms and prediction of physicochemical properties in cheminformatics. This can be seen most clearly in Quantitative Structure-Activity Relationships (QSAR), Quantitative Structure-Property Relationships (QSPR) and virtual screening methods[9,10], which all assume that the structure of a compound can determine its physical and chemical properties. These models use topological descriptors and molecular fingerprints based on graphs, which underlines their relevance to chemical sciences and the comprehension of molecules' behaviour.

Regarding the intersection of graph theory and chemistry, their relationship has existed since the former was employed to solve problems regarding the classification of isomers[11]. The development of topological indices, such as the Wiener index, has further strengthened this connection by providing a quantitative measure of molecular topology related to several physicochemical properties. New topological indices have now been proposed, which show new possibilities for the representation and analysis of complicated molecular substances[12,13]. It is inescapable that graph theory and chemistry are progressing together, and there is an ever-increasing scope of their interrelations; it is sufficient to say that in the study of molecular phenomena, graph theory is and will be of great importance[14,15].

The Zagreb indices are calculated for a set of unsaturated fatty acids, namely Myristoleic acid, Palmitoleic acid, Sapienic acid, Oleic acid, Elaidic acid, Vaccenic acid, Gadoleic acid, Eicosenic acid, and Erucic acid[16,17,18,19]. These unsaturated fatty acids are necessary for various metabolic and physiological activities[20]. This study aims to determine how the bond distance and the number of branches interact and correlate to the various metabolic functions of the molecules in question. In addition, the study of geometric properties of these commercially available fatty acids[21] serves transformational goals in explaining how structures of molecules influence energy metabolism. These insights shed more light on the metabolism of fatty acids and demonstrate graph theory as a spanner in solving scientific problems and fostering interdisciplinary study development[22].

Methodology

This study aims at the investigation of degree-based Zagreb indices such as First Zagreb Index (M_1)[23], Second Zagreb Index (M_2), First Hyper Zagreb Index (HM_1)[23] and Second Hyper Zagreb Index (HM_2) as well as their relationships with the properties of certain unsaturated acids. The degree-based variants of these indices provide for an elaborated consideration of the complexity of the molecular architecture.

The indices are computed as follows:

$$M_1 = \sum_{u,v \in G} (d_u + d_v) \quad (1)$$

$$M_2 = \sum_{u,v \in G} (d_u\, d_v) \quad (2)$$

$$HM_1 = \sum_{u,v \in G} (d_u + d_v)^2 \quad (3)$$

$$HM_2 = \sum_{u,v \in G} (d_u d_v)^2 \quad (4)$$

Here, G denotes the collection of edges in the graph G and d_u and d_v represent the degrees of the vertices u and v, respectively.

While calculating and determining these indices, the following steps were followed:

1. **Selection of Unsaturated Fatty Acids**: The fatty acids that were selected for the analysis included Myristoleic acid, Palmitoleic acid, Sapienic acid, Oleic acid, Elaidic acid, Vaccenic acid, Gadoleic acid, Eicosenoic acid and Erucic acid[18,19].
2. **Graph Representation:** The molecular structure of these fatty acids was represented by graphs where atoms are a vertex in the graphs and the bonds are the edges.
3. **Computation of Indices:** The selected Zagreb indices were calculated using the SPSS software. The indices were computed from the degree sequences of the molecular graphs.
4. **Physicochemical Properties:** The four physicochemical properties selected for correlation analysis were-LogP, Enthalpy, Molar Refraction and Polarizability[20].
5. **Linear Regression Analysis:** The relationship between the computed Zagreb indices and the selected physicochemical properties was studied based on linear regression. Both intercept and slope 95% of the significance level were calculated for confidence interval to test the validity of the models.
6. **QSPR Model Construction:** QSPR models were established to determine the relationship between the Zagreb indices and the structural characteristics of unsaturated fatty acids.[8,10]

Thus, employing such methods, the study seeks to appreciate the effectiveness of degree-based Zagreb indices in indicating the physicochemical characteristics of unsaturated fatty acids and, thus, their metabolism and physiological functions. This approach underlines the usefulness of graph theory in chemical research and its capacity to solve intricate problems in science.

RESULTS AND DISCUSSIONS

The paper begins by introducing the concept of Zagreb indices and their application to predicting the physicochemical properties of unsaturated fatty acids. Fig. 1 showcases the molecular structures of the studied fatty acids, providing a visual representation of their topological features. Following this, Table 1 presents the degree-based edge partitioning and M-polynomials for each fatty acid, highlighting the number of atoms, bonds, and key polynomial expressions.

Table 2 lists the physicochemical properties, including enthalpy, polarization, LogP, and molar volume, which are essential for understanding the relationships between molecular structure and properties. These properties form the basis for correlation analysis with the computed Zagreb indices.

Table 3 provides the calculated values for the 1st and 2nd Zagreb indices, as well as their hyper variants, which quantify the structural complexity and branching of the fatty acids. The correlation coefficients between these indices and the physicochemical properties are presented in Table 4, demonstrating strong predictive relationships, especially for properties like polarization, LogP, and molar volume.

The statistical properties of the regression models, such as constants, slopes, correlation coefficients, and significance levels, are detailed in Tables 5 through 8. These tables highlight the predictive accuracy of the models and underscore the statistical significance of the relationships. Table 9 summarizes the standard error of estimates for the physical properties, further validating the QSPR models.

The visual correlation between physical properties and Zagreb indices is illustrated in Fig. 2, while Fig. 3 graphically represents the relationships between the indices and properties like enthalpy and molar volume. This cohesive flow of data and visualizations reinforces the study's conclusion that Zagreb indices are highly effective in modeling and predicting the physicochemical properties of unsaturated fatty acids.

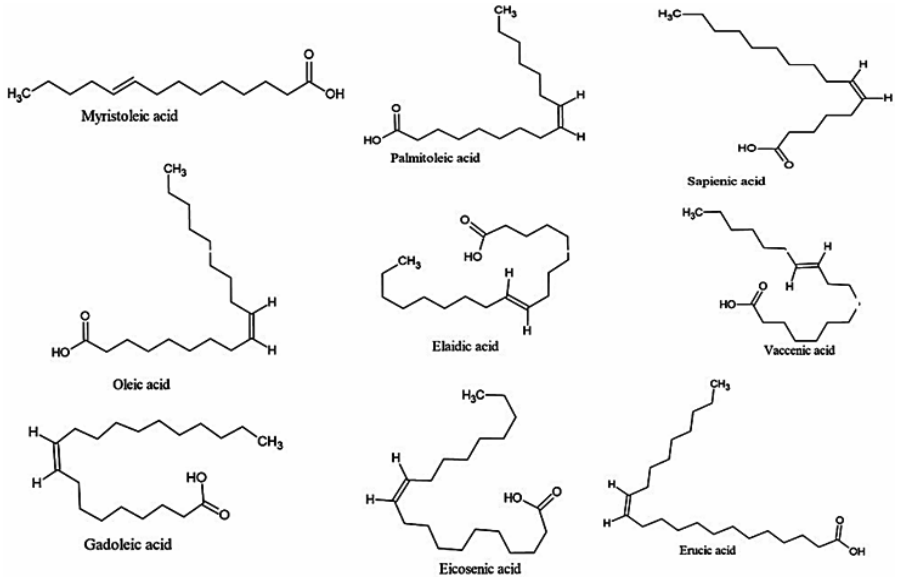

Fig. 1. Chemical Structures of Unsaturated Fatty Acids

Table 1: Degree-Based Edge Partitioning of Unsaturated Fatty acids and Their M-Polynomials

Compounds	Atoms	Bonds	d1,2	d2,2	d2,3	d3,1	M(G;x,y)
Myristoleic acid	16	15	1	11	1	2	$xy^2+11x^2y^2+x^2y^3+2x^3y$
Palmitoleic acid	18	17	1	13	1	2	$xy^2+13x^2y^2+x^2y^3+2x^3y$
Sapienic acid	18	17	1	13	1	2	$xy^2+13x^2y^2+x^2y^3+2x^3y$
Oleic acid	20	19	1	15	1	2	$xy^2+15x^2y^2+x^2y^3+2x^3y$
Elaidic acid	20	19	1	15	1	2	$xy^2+15x^2y^2+x^2y^3+2x^3y$
Vaccenic acid	20	19	1	15	1	2	$xy^2+15x^2y^2+x^2y^3+2x^3y$
Gadoleic acid	22	21	1	17	1	2	$xy^2+17x^2y^2+x^2y^3+2x^3y$
Eicosenic acid	22	21	1	17	1	2	$xy^2+17x^2y^2+x^2y^3+2x^3y$
Erucic acid	24	23	1	19	1	2	$xy^2+19x^2y^2+x^2y^3+2x^3y$

Table 2: Physicochemical Properties of Unsaturated Fatty acids

Unsaturated fatty acid	Enthalpy	Polarization	LogP	Molar volume
Myristoleic acid	64.0	27.2	5.57	247.9
Palmitoleic acid	67.0	30.8	6.64	280.9
Sapienic acid	67.7	30.8	6.70	280.9
Oleic acid	66.5	34.5	7.70	313.9
Elaidic acid	66.5	34.5	7.70	313.9
Vaccenic acid	71.2	34.5	7.70	313.9
Gadoleic acid	71.8	38.2	8.76	346.9
Eicosenic acid	74.7	38.2	8.76	346.9
Euric acid	69.7	41.9	9.82	379.9

Table 3: Topological Indices of Unsaturated Fatty acids

Acids	1st Zagreb	2nd Zagreb	1st hyper Zagreb	2nd hyper Zagreb
Myristoleic acid	60	58	3600	3364
Palmitoleic acid	68	66	4624	4356
Sapienic acid	68	66	4624	4356
Oleic aid	76	74	5776	5476
Elaidic acid	76	74	5776	5476
Vaccenic acid	76	74	5776	5476
Gadoleic acid	84	82	7056	6724
Eicosenic acid	84	82	7056	6724
Euric acid	92	90	8464	8100

We considered the linear regression model, $P = \alpha_i(TI) + \gamma$, to obtain the best relationship between the topological indices and the physicochemical properties of unsaturated fatty acids. Here, *P* is the physical property, and TI is the topological descriptor. γ and α_i denote the constant and the coefficients, respectively[24]. Using the data from Table 2 for the properties and Table 3 for the proposed indices after fitting and analysing the linear regression model defined by this equation for the physicochemical properties, the following key observations were made regarding the linear regression models.

1st Zagreb	2nd Zagreb
Enthalpy=0.2417(M_1)+50.42	Enthalpy=0.2417(M_2)+50.91
Polarization=0.4604(M_1)-0.4806	Polarization=0.4604(M_2)+0.4403
LogP=0.1321(M_1)-2.333	LogP=0.1321(M_2)-2.069
Molar Volume=4.125(M_1)+0.4000	Molar Volume=4.125(M_2)+8.650
1st Hyper Zagreb	**2nd Hyper Zagreb**
Enthalpy=0.001549(HM_1)+59.71	Enthalpy=0.001589(HM_2)+59.95
Polarization=0.003016(HM_1)+16.83	Polarization=0.003097(HM_2)+17.29
LogP=0.0008648(HM_1)+2.637	LogP=0.0008880(HM_2)+2.767
Molar Volume=0.02701(HM_1)+155.6	Molar Volume=0.02774(HM_2)+159.6

Table 4: Correlation Coefficients of Physical Properties

Topological Index	Correlation Coefficient of Enthalpy	Correlation Coefficient of Polarization	Correlation Coefficient of LogP	Correlation Coefficient of Molar Volume
1st Zagreb	0.712117	0.999983	0.99987729	1
2nd Zagreb	0.712117	0.999983	0.999877	1
1st hyper Zagreb	0.69522	0.997999	0.997384	0.9977
2nd hyper Zagreb	0.69472	0.997882	0.997253	0.997574

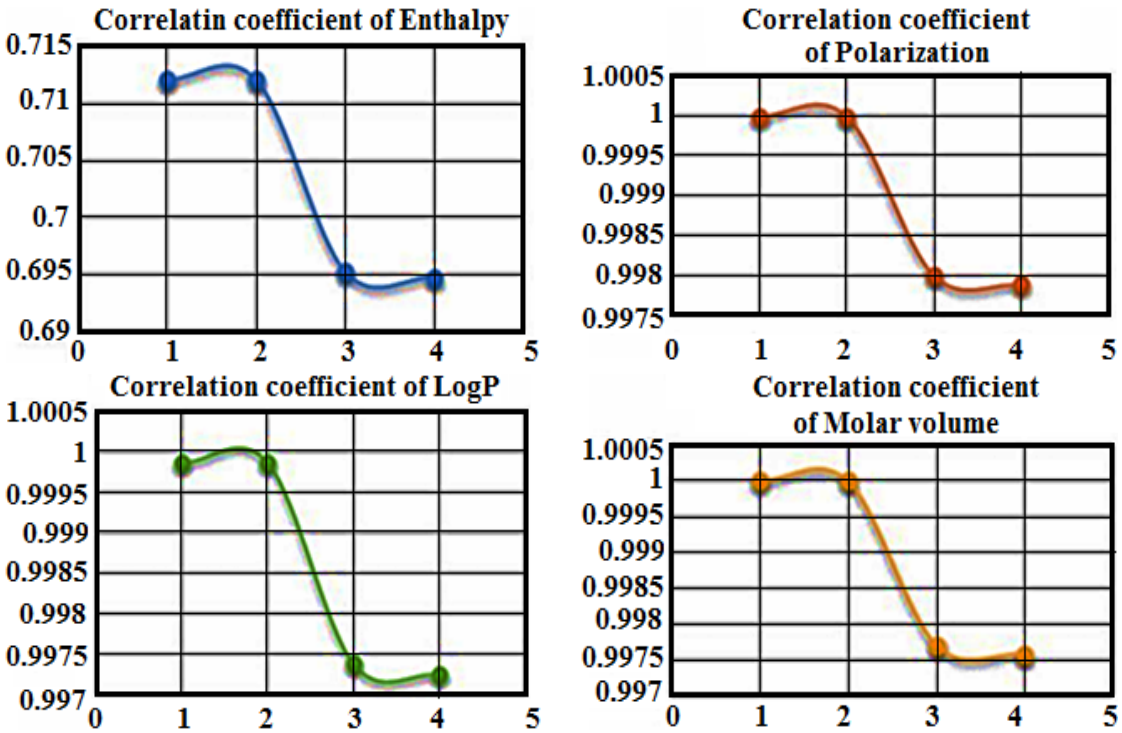

Fig. 2. Correlation between physical properties of drugs and topological indices

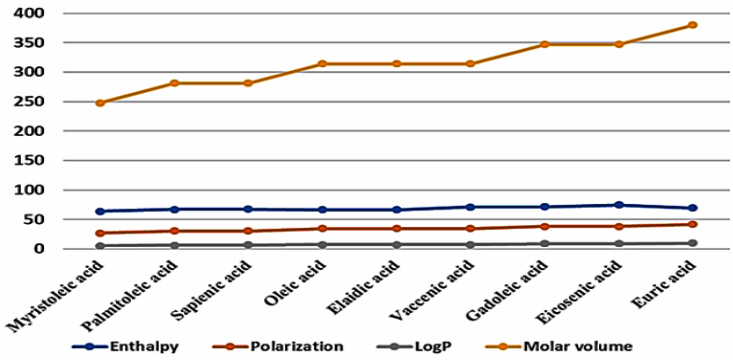

Fig. 3. Graph of properties with topological indices

Table 5: Statistical Properties for 1st Zagreb

Physical Property	N	A	B	r	r^2	F	Indicator
Enthalpy	9	50.42	0.2417	0.7121	0.5071	7.201957	Significant*
Polarization	9	- 0.4806	0.4604	0.99998	0.99996	205132.2	Significant**
LogP	9	- 2.333	0.1321	0.9999	0.9998	28517.15	Significant**
Molar volume	9	0.4000	4.125	1	1	8.63E+31	Significant**

*Significant at 5% level and ** Significant at 1% level

Table 6: Statistical Properties for 2nd Zagreb

Physical property	N	A	B	r	r^2	F	Indicator
Enthalpy	9	50.91	0.2417	0.7121	0.5071	7.201957	Significant*
Polarization	9	0.4403	0.4604	0.9999	0.9998	205132.2	Significant**
LogP	9	- 2.069	0.1321	0.9998	0.9996	28517.15	Significant**
Molar volume	9	8.650	4.125	1	1	8.63E+31	Significant**

Table 7: Statistical Parameters for 1st hyper Zagreb

Physical properties	N	A	B	r	r^2	F	Indicator
Enthalpy	9	59.71	0.001549	0.6952	0.4833	6.5483	Significant*
Polarization	9	16.83	0.003016	0.9979	0.9958	1744.172	Significant**
LogP	9	2.637	0.0008648	0.9973	0.9946	1332.621	Significant**
Molar volume	9	155.6	0.02701	0.9977	0.9954	1516.2	Significant**

Table 8: Statistical Parameters for 2nd hyper Zagreb

Physical property	N	A	B	r	r^2	F	Indicator
Enthalpy	9	59.95	0.001589	0.6947	0.4826	6.530136	Significant*
Polarization	9	17.29	0.003097	0.9978	0.9957	1647.481	Significant**
LogP	9	2.767	0.0008880	0.9972	0.9945	1268.938	Significant**
Molar volume	9	159.6	0.02774	0.9975	0.9951	1437.45	Significant**

Table 9: Standard Error of Estimate

Topologicalindex	Enthalpy	Polarization	LogP	Molar Volume
M1(G)	1.834553	5.174959	8.197032	28.78828
M2(G)	1.737965	4.952859	7.965724	29.01788
HM1(G)	721.831	725.6528	728.6427	694.6043
HM2(G)	686.4214	690.2323	693.2138	659.281466

*Significant at 5% level and **Significant at 1% level

CONCLUSION

This work introduces significant improvements related to Zagreb descriptors and their combinations, which better approximate the physicochemical properties of unsaturated fatty acids. The results demonstrate the substantial performance enhancement of the newly defined hybrid descriptors over the classical indices. This advancement significantly expands the scope of utilization of topological indices in the modelling of QSPR.

Our QSPR models, based on linear regression, successfully predicted the values of interest, particularly properties like polarization, LogP, and molar volume. However, the correlation of the models with the enthalpies of formation in the gas phase was not as successful, underscoring the need for further refinements in QSPR models. This ongoing research is crucial to address the complexities associated with various aspects related to enthalpy prediction for unsaturated fatty acids.

Regardless, our results provide a promising platform for future systematic work to overcome these challenges. With improved QSPR models, we can expect enhanced predictions of enthalpy and other physicochemical properties. These advancements will significantly boost the scientific community's ability to study and predict the properties of unsaturated fatty acids, potentially revolutionizing fields such as biochemistry, drug development, and nutrition science.

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Conflict of interest

The author declare that we have no conflict of interest.

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