STM JOURNALS

Journal of
Polymer & Composites

ISSN: 2321-2810 (Online)
ISSN: 2321-8525 (Print)
Volume 14, Special Issue 1, 2026
DOI (Journal): 10.37591/JoPC

https://journals.stmjournals.com/jopc

Review JoPC

Graph Theoretic Analysis of Cyclodextrin Polymers

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Abstract

Topological indicators in chemical graph theory are essential tools in cheminformatics, providing valuable insights into molecular structure and properties to make more accurate predictions about the behavior and efficacy of novel compounds in drug design. The macro molecules are correlated with certain derivatives. The derivatives are growing structures which depends on the cyclic structures. The Cyclodextrin is one of the cyclic structures which depends on the carbon atoms. The polymer derivatives are growth of network which raising the carbon atoms and connection between the bonds. The Cyclodexstrin is one of the polymer structure which was gradually increase th carbon atoms. Cyclodextrin derivatives represent in polymer chemistry, as they combine the unique inclusion properties of cyclodextrins with the tunable characteristics of polymers. These derivatives can form polymeric networks through various mechanisms, including covalent bonding, non-covalent interactions, and supramolecular assembly. Incorporating CDs into polymers significantly enhances solubility, stability, and binding selectivity. This research investigates the relationship between various physicochemical properties of cyclodextrin derivatives for complexity, polar surface area, melting point, and boiling point used topological descriptors for the first and second zagreb indices. The Cyclodextrin derivatives obtained the topological indices and correlate with their physico chemical properties The linear regression models were analysed.

Keywords: Topological index, valency, cyclodextrin derivatives, molecules, polymers.

INTRODUCTION

Chemical graph theory is a mathematical chemistry, the chemical structure representing the molecular graph. The connections between the bonds such as single bond, double bond or triple bond can be treated as edges connecting to the vertices. In the molecular graph, vertices are connected to the atoms and degree of the vertices as valence of the atoms. The molecular properties predict biological activity, and design drugs optimally by employing mathematical methods. Topological indices are the numerical descriptors computed from molecular graphs [3]. Molecule measures assist in comparing molecules with established drugs to find new candidates. Substructure and motif identification in molecular graphs support ligand identification [4,7]. The topological indices expect residences together with Solubility, Lipophilicity (log P), toxicity, and metabolism. Quantitative graph-theoretic methods, particularly the $\mathcal{M}$-polynomials, are employed to systematically assess the structural features of cyclodextrin polymer derivatives [8,9]. These methods support advancements in drug delivery systems by optimizing drug formulations and improving the efficacy of cyclodextrin-based treatments [14–16]. The findings are expected to contribute significantly to the development of novel drug delivery platforms, addressing common challenges such as poor drug solubility [9]. Understanding drug–cyclodextrin interactions is essential for maximizing the therapeutic potential

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Received Date: September 05, 2025
Accepted Date: December 01, 2025
Published Date: February 09, 2026

Citation: N. Kumaran, J. Senbagamalar, S. Gayathri and A. Vijayalakshmi. Graph Theoretic Analysis of Cyclodextrin Polymers. Journal of Polymer & Composites. 2026; 14(Special Issue 1): S997–S1006p.

of such systems [1,6]. The design of cyclodextrin-based drug delivery systems tailored to specific therapeutic needs can ultimately lead to enhanced patient outcomes in clinical settings. Therefore, this research underscores the critical role of cyclodextrin's structural properties in pharmaceutical formulation and highlights the need for continued investigation into its derivatives to revolutionize drug delivery and therapeutic efficacy across various medical fields.

Application of Topological Indices to Cyclodextrin Derivatives

Cyclodextrin derivatives (CD) in drug studies possess a unique ability to encapsulate a wide range of drugs, thereby enhancing their solubility and stability [2]. Physico-chemical characterization and their application are characterized in [17–21]. Supramolecular polymers containing cyclodextrins are primarily based on host–guest interactions, where the CD cavity encapsulates hydrophobic polymer side chains such as adamantane, azobenzene, and ferrocene. The reversible and dynamic nature of these interactions enables the development of self-healing systems, stimuli-responsive gels, and smart coatings. Applications of CD-based polymers are diverse. In drug delivery, they improve the solubility of poorly soluble drugs and facilitate controlled release through polymer matrices. In environmental remediation, they serve as efficient adsorbents for dyes, pollutants, heavy metals, and pesticides. In tissue engineering and biomedical fields, CD-based hydrogels are employed in wound healing, while gene delivery systems also benefit from their functional versatility.

Under the category of smart materials, responsive hydrogels demonstrate sensitivity to pH, temperature, redox, and light stimuli, whereas slide-ring elastomers exhibit remarkable stretchability. Finally, in catalysis and separation science, CD derivatives are crucial for enzyme immobilization, molecular recognition, and the design of separation membranes. Topological indices provide numerical representations of the structural properties inherent in molecular graphs. In the case of cyclodextrin (CD) derivatives, degree-based indices are particularly effective for assessing branching and connectivity in CD rings and their substituted derivatives. Comparative studies involving different substituents (–OH, $–CH_3$, $–CH_2CH_2OH$) highlight their influence on molecular connectivity. Distance-based indices successfully capture the ring size variations among α-, β-, and γ-CD, thereby enabling correlations between cavity size and host–guest interaction properties. Eccentricity-based indices offer insights into molecular compactness and symmetry, with derivative substitutions altering eccentricities by modifying local environments.

Recently developed indices can be applied to functionalized CDs, facilitating the investigation of structure–property relationships such as enhanced solubility and increased binding affinity toward hydrophobic guests. The stability of supramolecular polymers based on CDs is also of significant interest. Structure–property correlations provide a framework for linking CD-based topological indices to drug delivery performance, including solubility enhancement and drug binding strength. Polymer stability, particularly the resistance of CD crosslinked networks, is crucial for applications in environmental remediation and for improving the adsorption efficiency of pollutants. In biomedical applications, diffusion behavior in CD-based hydrogels warrants particular attention.

From a research perspective, comparative TI studies can be employed to explore and contrast α-, β-, and γ-CD and their derivatives. Furthermore, supramolecular inclusion complexes involving CD–drug or CD–polymer systems can be represented using graph-theoretic operations such as graph joins or corona products, thus enabling the derivation of novel formulations of topological indices. The development of CD-specific indices capable of capturing cavity size, degree of substitution, and molecular symmetry would represent a groundbreaking contribution to the field, offering deeper insight into the structural and functional diversity of cyclodextrin derivatives.

$\mathcal{M}$-Polynomial on Topological Indices

Polynomials are important in the study of topological indices with respect to chemical graph theory. $\mathcal{M}$-polynomials were first introduced as a systematic approach to a unifying idea, and are generating functions representing edge-based structural information of molecular graphs [5]. The M-polynomial

of a graph $\mathcal{H}$ is defined as $\mathcal{M}(\mathcal{H}; p, q) = \sum_{i \leq j} P_{ij} p^i q^j$, Here P_{ij}, represents the number of edges in $\mathcal{H}$ connecting degree i vertices to degree j vertices. The M-polynomial enables the researcher to obtain from it most of the degree-based topological indices including, the Zagreb indices, Randić index, and the harmonic index, by suitable mathematical modifications of the polynomial.

In 2021, Mondal et al presents some significant findings about the application of ensemble learning and graph topological indices towards predicting the physical properties of mental disorder drugs [10]. One of the functions of $\mathcal{M}$-polynomials in the study of chemical structures is to make it possible to predict physicochemical properties and biological activities from topological indices in a mathematical model that generalizes molecular graphs and their intricate molecular structure and branchings and connectivity. $\mathcal{M}$ -polynomials form a convenient basis in theoretical chemistry and quantitative structure-activity relationships (QSAR) [11].

The $\mathcal{M}$-polynomials to be an efficient and general method of obtaining numerous degree-based topological indices from the molecular graph of a compound. For alkanes the $\mathcal{M}$-polynomial can encode connectivity information regarding the carbon. Consider an alkane such as butane, the molecular graph has carbon atoms connected by single bonds, but each bond connects vertices of particular degree.

Once we have the $\mathcal{M}$-polynomial calculated, it is possible to deduct important topological indices. This analytical approach offers computational effectiveness for the computation of several indices from a vast molecular graph, and also offers the potential to model QSAR and structure more effectively throughout drug discovery, material science, and nanotechnology [12, 13].

The $\mathcal{M}$ -polynomials offer a single method of calculation and investigation of degree-based topological indices, and they are well known within chemical graph theory and quantitative structure–activity relationship (QSAR) research. The degree based topological indices are $M_1(\mathcal{H}) = \sum_{uv \in E(\mathcal{H})}(\delta_u + \delta_v)$, $M_2(\mathcal{H}) = \sum_{uv \in E(\mathcal{H})}(\delta_u * \delta_v)$ where δ_u be the degree of the vertex u in $\mathcal{H}$. Channakrishnappa et al examines the $\mathcal{M}$-polynomial and Neighborhood M-polynomial of four antiviral agents, A-315675, Oseltamivir Carboxylate, Zanamivir, and BCX-1812. $\mathcal{M}$ -polynomials offer systematic approaches toward computing indices - both obtaining degree-based indices and general enthusiasts in those fields that quantify the frequency of edges between atoms of varying degrees, the Zagreb indices, Randić index, harmonic index or inverse sum index.

Instead of computing each index separately, the $\mathcal{M}$-Polynomial acts as a generating function from which all of these indices can be calculated through differentiation and coercive algebraic procedures. $\mathcal{M}$-polynomials are not just a computationally efficient way of calculating topological indices, they have been successfully used in practical applications in order better understand the structural properties of drugs, predict biological activity, monitor molecular stability, in the classification of chemical compounds. $\mathcal{M}$ -polynomials have efficiently blended into cheminformatics and drug discovery pipelines.

In this research, correlation and regression analyses are performed for cyclodextrin derivatives to examine the relationship between the First and Second Zagreb Indices and their physicochemical properties.

METHODOLOGY

Cyclodextrins CDs are ring oligosaccharides connected with units linked by α-1,4-glycosidic bonds and generally produce a toroidal shape. The α-, β-, and γ-cyclodextrin contain 6, 7, and 8 glucose units, respectively. To expand the physicochemical characteristics, applicability within the pharmaceutical realm, numerous cyclodextrin derivatives have been synthesized through various chemical modifications.

Using M polynomial, calculating the first Zagreb index

$$M_1(\mathrm{H})=\sum_{uv\in E(\mathrm{H})}(\delta_u+\delta_v)=(D_u+D_v)\wp(u,v)|_{u=v=1}$$

$M_2(\mathrm{H})=\sum_{uv\in E(\mathrm{H})}(\delta_u\delta_v)=(D_uD_v)\wp(u,v)|_{u=v=1}$, where $D_u=u\frac{\partial}{\partial u}$ and $D_v=v\frac{\partial}{\partial v}$

The M-polynomial for cyclodextrin α-CD is

$$\wp(u,v)=38u^2v^3+16u^3v^3+8uv^3+6u^2v$$

The M-polynomial for cyclodextrin β-CD is

$$\wp(u,v)=35u^2v^3+28u^3v^3+21uv^3$$

The M-polynomial for cyclodextrin γ-CD is

$$\wp(u,v)=40u^2v^3+32u^3v^3+16uv^3+8u^2v$$

Calculating first Zagreb index for cyclodextrin α-CD, using M-polynomial is

$$\wp(u,v)=38u^2v^3+16u^3v^3+8uv^3+6u^2v$$

$$D_u=u\frac{\partial}{\partial u}\wp(u,v)=\left(76u^2v^3+48u^3v^3+8uv^3+12u^2v\right)$$

$$D_v=v\frac{\partial}{\partial v}\wp(u,v)=\left(114u^2v^3+48u^3v^3+24uv^3+6u^2v\right)$$

$$M_1(\mathrm{H})=\sum_{uv\in E(\mathrm{H})}(\delta_u+\delta_v)=(D_u+D_v)\wp(u,v)|_{u=v=1}$$

$$M_1(\mathrm{H})=\left[\left(76u^2v^3+48u^3v^3+8uv^3+12u^2v\right)+\left(114u^2v^3+48u^3v^3+24uv^3+6u^2v\right)\right]\Big|_{u=v=1}$$

$$M_1(\mathrm{H})=336$$

Calculating second Zagreb index for cyclodextrin α-CD, using M-polynomial is

$$\wp(u,v)=38u^2v^3+16u^3v^3+8uv^3+6u^2v$$

$$D_v=v\frac{\partial}{\partial v}\wp(u,v)=\left(114u^2v^3+48u^3v^3+24uv^3+6u^2v\right)$$

$$D_u(D_v)=228u^2v^3+144u^3v^3+24uv^3+12u^2v$$

$$M_2(\mathrm{H})=\sum_{uv\in E(\mathrm{H})}(\delta_u\delta_v)=(D_uD_v)\wp(u,v)|_{u=v=1}$$

$$M_2(\mathrm{H})=208$$

In this manner, calculate the first zagreb index and secon zagreb index for cyclodextrin β-CD and cyclodextrin γ-CD are shown in Table 1. The cyclodextrin derivatives of Figure 1,2 and 3 are taken from Pub Chem and their physico chemical properties are shown in Table 1. The branching features inherent in the molecular graph are represented by a topological index based on degree. The

Second Zagreb Index exhibits an upward trajectory from α to γ-cyclodextrin (CD), denoting an augmentation in the molecular branching and complexity of the graph's structural arrangement. γ-CD, which presents the highest quantitative value, is characterized by the most intricate connectivity among the trio of compounds.

Table 1. The first and second Zagreb index values and physicochemical properties for cyclodextrin derivatives

Drugs	M_1(H)	M_2(H)	Polar Surface Area A^2	Complexity	Melting point	Boiling point	Molar Volume
cyclodextrin α-CD	336	208	475	1250	278	784	--
cyclodextrin β-CD	427	525	554	1480	290	1541	698
cyclodextrin γ-CD	436	592	633	1720	267	474	4.27

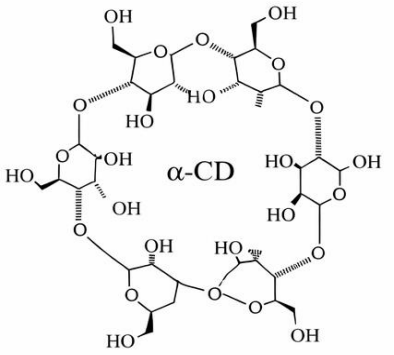

Figure 1. The molecular structure cyclodextrin α-CD

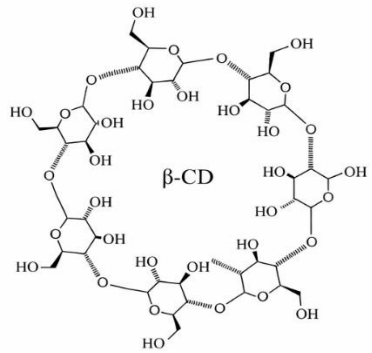

Figure 2. The molecular structure cyclodextrin β-CD

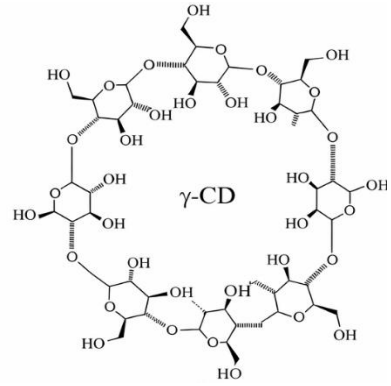

Figure 3. The molecular structure cyclodextrin γ-CD

To predict pharmaco kinetic characteristics like permeability and absorption, the majority of the surface area covered by polar atoms is used. The polar surface area increases as the dimensionality of the cyclodextrin increases. An elevated PSA, as observed in γ-CD, frequently correlates with enhanced aqueous solubility, although it may concurrently lead to diminished membrane permeability unless subject to modification. Combining several characteristics, such as atom types, ring systems, and branching geometries, results in a structural descriptor values.

The number of glucose units increases from α to γ (6, 7, and 8, respectively), leading to a rise in structural complexity Elevated complexity may influence the challenges associated with synthesis and the reactivity of the compounds. β-CD exhibits the highest melting point, indicating superior thermal stability. The lower melting temperature of γ-CD, despite its increased complexity, may be explained by its looser molecular packing. The boiling point of β-CD is unusually high compared to other CDs, which probably means that there is strong intermolecular hydrogen bonding.

Because γ-CD has a somewhat lower boiling point, it may be more volatile in certain circumstances β-CD is characterized by the largest molar volume, implying increased available space within its cavity for the encapsulation of therapeutic agents. The value associated with γ-CD is notably small and may necessitate further validation, as it appears anomalously low in relation to the prevailing trend.

CORRELATION ANALYSIS FOR CYCLODEXTRIN DERIVATIVES

The Strong Positive Correlations in polar surface area r = 0.904, complexity r = 0.899. These values indicate that the first Zagreb index is highly correlated with the molecules have higher Zagreb values tend to have a greater polar surface, suggesting that more connected or branched structures expose more polar atoms as in Table 2. The molecular complexity is strong correlation confirms that the first Zagreb index effectively captures the structural intricacies of cyclodextrins.

The weak or negligible correlations are melting point r = –0.056, boiling point r = 0.155. These low correlations shows that the first Zagreb index does not significantly predict thermal properties like melting or boiling point. The topological connectivity are not sufficient to infer thermal behavior. The strong negative correlation is flash point r = –0.969. This very strong inverse correlation implies that as the first Zagreb index increases, the flash point decreases, potentially signaling that more complex and branched. cyclodextrins may have lower ignition temperatures and could pose greater flammability risks. The moderate correlations in molar refractivity is r = –0.456, moderately negative. The molar volume r = 0.433 is moderately positive. The first Zagreb index has a modest positive correlation with molecular size and volume. A negative relationship with refractivity might suggest that more branched molecules may not align linearly with electronic polarizability.

Table 2. The correlation matrix for first Zagreb index

Properties	First Zagreb index	Polar Surface Area	Complexity	Melting point	Boiling point	Flash point	Molar Refractivity	Molar Volume
First Zagreb index	1.000							
Polar Surface Area	0.904	1.000						
Complexity	0.899	1.000	1.000					
Melting point	-0.056	-0.478	-0.489	1.000				
Boiling point	0.155	-0.282	-0.294	0.978	1.000			
Flash point	-0.969	-0.982	-0.979	0.302	0.095	1.000		
Molar Refractivity	-0.456	-0.793	-0.800	0.914	0.809	0.662	1.000	
Molar Volume	0.433	0.005	-0.007	0.876	0.958	-0.196	0.605	1.000

The First Zagreb index is an excellent indicator of molecular complexity and polar surface area, validating its utility in graph-theoretic modeling. It does not predict melting points and boiling points effectively. A notable negative correlation with flash point implies a potential link between topological complexity and chemical safety concerns. Its moderate correlation with molar volume supports its partial use in size-related estimations, though not as strongly as the second Zagreb index.

As in Table 3, Second Zagreb Index, molar volume r = 0.357 which is weak and moderate, molar refractivity r = 0.605 which moderate, melting Point r = 0.875 which is strong positive correlation. The graph-theoretic indices like the second Zagreb index are strong indicators of cyclodextrin molecular structure complexity, PSA. Thermal properties such as melting points and boiling points are highly influenced by both molecular size (molar volume) and electronic properties. The flash point shows inverse relationships with nearly all other descriptors, suggesting that as cyclodextrins become structurally complex, their flammability increases. The nearly perfect correlation between complexity and polar surface area shows that PSA can be predicted directly from structural/topological analysis.

LINEAR REGRESSION ON FIRST AND SECOND ZAGREB INDICES

The linear equation $y = mx + c$ delineates the correlation between the explanatory variable and the dependent variable, with m representing the slope and c denoting the intercept.

Table 3. The correlation matrix for second Zagreb index

Properties	Second Zagreb index	Polar Surface Area	Complexity	Melting point	Boiling point	Flash point	Molar Refractivity	Molar Volume
Second Zagreb index	1.000							
Polar Surface Area	0.936	1.000						
Complexity	0.932	1.000	1.000					
Melting point	-0.139	-0.478	-0.489	1.000				
Boiling point	0.073	-0.282	-0.294	0.978	1.000			
Flash point	-0.986	-0.982	-0.979	0.302	0.095	1.000		
Molar Refractivity	-0.527	-0.793	-0.800	0.914	0.809	0.662	1.000	
Molar Volume	0.357	0.005	-0.007	0.876	0.958	-0.196	0.605	1.000

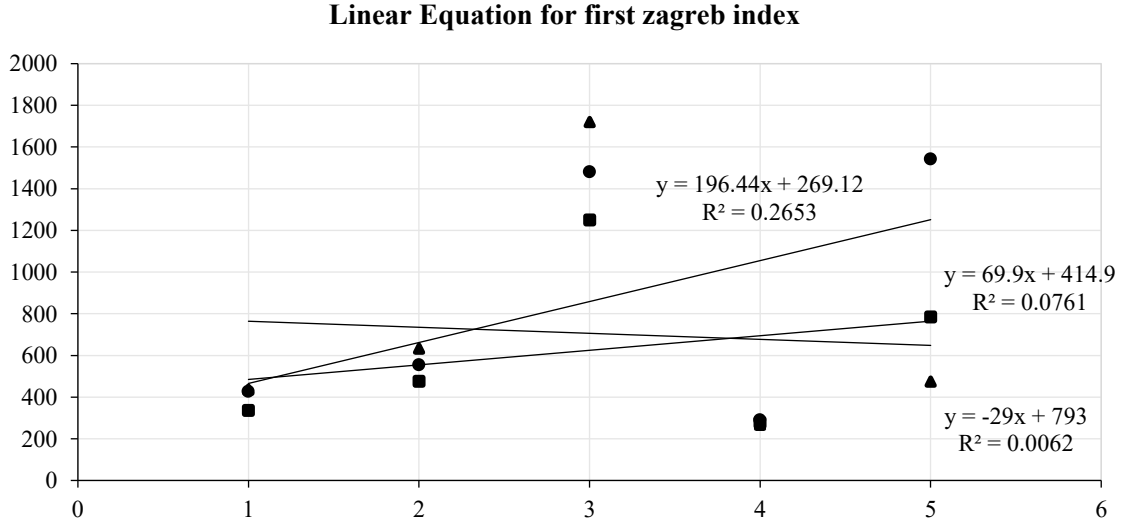

Figure 4. The trend lines on first zagreb index

The First Zagreb index and corresponding chemical properties such as polar surface area, complexity, melting point, and boiling point), is a detailed theoretical approach, along with the identification of the best-fitting linear equation in "Figure"4.

The First Zagreb index in Table 4 is based on vertex degrees increases, the molecular graph becomes more complex, often leading to a larger polar surface area due to more hydroxyl groups and branching. This makes sense chemically because CD derivatives with more glucose units will naturally have higher PSA. Both first zagreb index and complexity measure structural intricacies, complexity includes ring systems, heteroatoms, and topological features. Hence, the correlation is not strong. Melting point depends heavily on intermolecular forces, crystalline packing, and impurities, graph topology. Therefore, graph-based descriptors alone are insufficient for thermal behavior predictions.

As in "Figure" 5. the second zagreb index and its relationship with various chemical properties, the theoretical analysis and a conclusion about which linear equation provides the best fit.

The regression equations in Table 5, shows the different chemical properties relate to the second zagreb index on the topological index based on vertex degrees and adjacency, a useful measure of molecular branching and bond multiplicity in chemical graph theory. The highest coefficient of determination, meaning 22.7% of the variation in the dependent variable is explained by the Second Zagreb index. As the second Zagreb index increases, the property likely complexity or polar surface area also increases to positive correlations.

Table 4. Regression equation for first zagreb index

Property	Regression Equation	r^2 value	Interpretation
Polar surface Area	y=69.9x+414.9	0.6791	Good fit
Complexity	y=196.44x+269.12	0.2653	Moderate
Melting Point	y=−9x+793	0.0062	Very poor
Boiling Point	Not labeled but visible	Appears poor	Not reliable

Table 5. Regression equation for second zagreb index

Second zagreb index	Linear Equation	r^2 value	Interpretation
Polar surface area	y=176.84x+347.52	0.227	Weak to moderate
Melting point	y=95.5x+312.5	0.1251	Weak
Boiling point	y=−63.0x+917.8	0.0281	Very weak

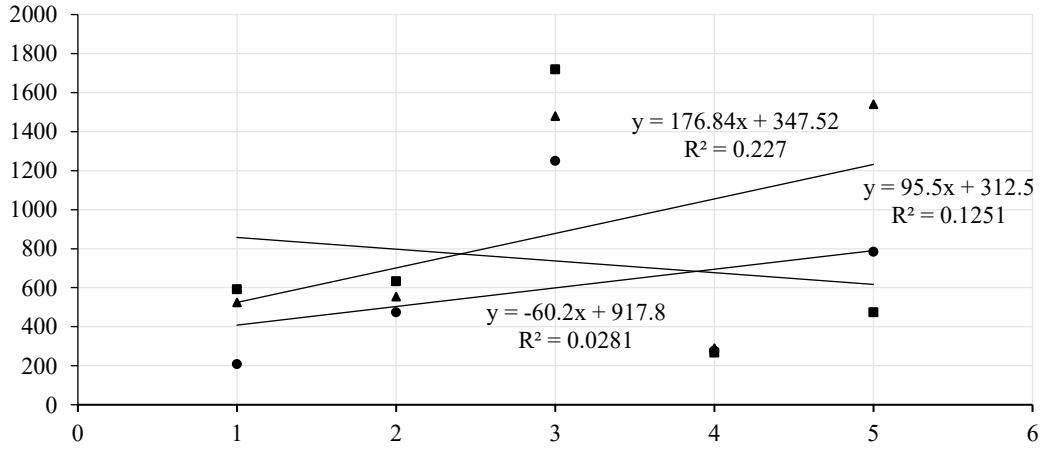

Figure 5. The trend lines on second zagreb index

The higher zagreb indices occurs more branching and complexity for larger surface area or complexity by 12.5% of variation is explained. The thermal property like melting point, which doesn't depend on molecular connectivity or structure. The Second Zagreb index alone is not a good predictor for this property. Only 2.8% of the variance is explained was basically no meaningful correlation. The negative slope might imply a very weak inverse relationship, but it is statistically irrelevant. The flash point or boiling point, which are influenced by multiple non-topological factors. The Second Zagreb index has the most predictive power for structural parameters like complexity or polar surface area, but not for thermal or volatility-related parameters.

CONCLUSION

This study examines the relationships between the first and second zagreb indices, two well-known topological descriptors, and a number of physicochemical characteristics of cyclodextrin derivatives, such as complexity, polar surface area, melting point, boiling point, flash point, molar refractivity, and molar volume. Although both indices work well as indicators of molecular branching and surface properties, they are less accurate at predicting thermal behavior, which is affected by variables like hydrogen bonding and crystal packing that are not well captured by simple topological descriptors.

The first zagreb index displays a stronger linear predictive capacity for key structural characteristics, such as polar surface area, even if both indices display similar correlation trends. The first zagreb index emerges as a superior linear predictor between the two, particularly concerning structural attributes such as polar surface area and complexity. Nonetheless, both indices fall short on their own for accurately modeling thermal characteristics, underscoring the necessity to integrate supplementary molecular descriptors for developing more comprehensive quantitative structure–activity relationship (QSAR) models in the realm of drug design.

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