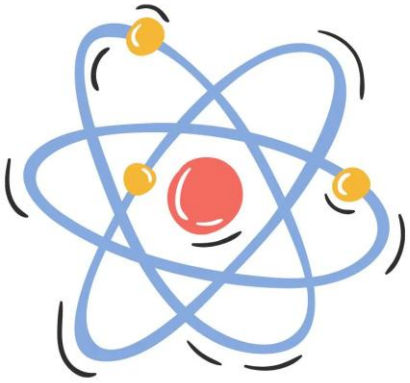

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Abstract: *Coumarins are polyphenolic compounds classified as colorless, crystalline oxygenated hetero- cyclic molecules. These are use used in the preparation of anti-cancer drugs. This research aims to explore the topological polynomials and indices of a series of drugs utilized in the treatment of cancer such as coumarins. A set of five degree based topological indices are considered, namely the first Zagreb index M1(G), the second Zagreb index M2(G), the second-order modified Zagreb index mM2(G), the redefined third Zagreb index ReZG3 and the forgotten index F (G) for the study. Further, the QSPR analysis revealed that the first Zagreb index is the potential topological index to predict physicochemical properties of coumarins.*

Keywords: *Coumarins, molecular graph, topological index, M-polynomial*

1. Introduction

Cancer is a leading cause of disease-related deaths globally. Although many chemotherapeutic agents have been developed to target uncontrolled cell division in various cancers, their use is often accompanied by severe side effects. Additionally, the emergence of multi-drug resis- tance poses a major challenge in anticancer therapy. Common symptoms of cancer include the formation of masses, abnormal bleeding, persistent cough, unexplained weight loss, and more. Key risk factors for cancer include tobacco use, obesity, poor dietary habits, physical inactivity, and excessive alcohol consumption. Treatment options for cancer include surgery, radiother- apy, chemotherapy, hormone therapy, targeted therapy, and other approaches. Among these, anticancer drugs, such as alkylating agents and metabolic modulators, play a critical role in managing the disease. Coumarins are polyphenolic compounds classified as colorless, crystalline oxygenated het- erocyclic molecules. They were first discovered by Vogel in 1820, when he isolated them from the Fabaceae plant Dipteryx odorata Willd, commonly referred to as ”coumaroun” [6, 7]. Oxy- genated heterocyclic compounds include furan derivatives, which contain 4 carbon atoms, and pyran derivatives, which contain 5 carbon atoms. While furan derivatives are relatively rare in plants, pyran derivatives are more abundant and serve as the structural foundation for various compounds, such as ketonic compounds like α-pyrones and γ-pyrones. In plants, the fusion of pyron derivatives with benzene results in the formation of secondary metabolites known as benzo-α-pyrones (coumarins) and benzo-γ-pyrones (chromones) [20, 23]. Chemical graphs serve as a non-numerical representation of chemical structures and are widely used in computing structural descriptors for QSAR/QSPR modeling [22, 30]. In this representation, chemical compounds are modeled as graphs, where atoms are represented as vertices and their corresponding bonds as edges. Typically, hydrogen atoms are omitted in chemical graphs. Topological indices have been demonstrated to contain substantial information regarding the three-dimensional structural properties of compounds [1, 16]. Chemistry serves as a fundamental foundation for the application of graph theory across various fields. Graphical invariants play a crucial role, offering a wealth of data that supports chemists in

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advancing their research. These graph invariants, also known as topological indices, predict a range of molecular properties of a compound by characterizing the graph topology of the molecule's structure [27, 28]. Topological graph measures are essential for quantitatively characterizing graphs. These measures can be classified into two main categories: information-theoretic and non-information- theoretic. They can also be further divided into graph invariants based on vertex degrees, dis- tances, eigenvalues, and other properties. Another classification includes symmetry measures, cyclicity measures, and branching measures. A vast number of topological graph measures have been developed and are widely applied in fields such as mathematical chemistry, bioinformatics, computer science, and more [33]. A significant number of drugs are developed annually and introduced to the market following clinical trials. Initially, extensive testing was required to identify side effects and toxicity in the human body, necessitating large laboratories and substantial resources. Researchers compared a vast array of compounds, analyzing their experimental results in relation to their molecular structures to determine drug properties. These properties are closely tied to the molecular structure of the compounds. In recent years, substantial progress has been made in the study of QSAR/QSPR modeling using the concept of topological descriptors [2, 5, 8, 25, 32]. Combining topological indices with hydrophobicity has led to the development of QSAR/QSPR relationships. Topological descrip- tors are utilized to differentiate between drug and non-drug compounds [10, 13]. These indices play a crucial role in identifying a large number of compounds in combinatorial syntheses and enabling the rapid screening of toxicity. Their popularity stems from their cost-effectiveness in designing effective drugs while minimizing the risks associated with new chemicals. Topological indices (TIs) have gained widespread recognition due to their ability to quickly compute and extract extensive information about the molecular structure of chemical compounds without the need for experimental procedures [31, 34, 35]. Changes in the chemical structure of organic compounds lead to systematic variations in their physicochemical properties and biological activities. Computational chemists focus on establishing quantitative relationships between structural features and properties to enable diagnostic and mechanistic interpretation or prediction of activities [23].

Topological indices assist chemists in determining whether a chemical compound should be included in a drug formulation based on the range of the index. Each index has a specific range, and if a compound exceeds the upper limit of this range, it is generally not recommended for inclusion in drug formulations intended for consumption by living organisms. Topological indices are valuable in QSPR studies, as they correlate physical properties with molecular structures.

Wiener was the first to apply the Wiener index in structure-property studies, discovering that it closely matched the boiling points of alkanes [19]. Numerous stud- ies have since utilized this index to establish connections between the physical and chemical properties of compounds, significantly advancing the application of graph theory in chemistry. In this work a set of coumarins were considered for the study and they were modeled as a molecular graphs. Consider a graph G = (V, E) with vertices V , represented as atoms and edges E represented as bond respectively. Refer [12] for standard notations and terminologies of graphs. Initially M-polynomials of five degree based topological indices were calculated for molecular graphs of coumarins. The indices are M1(G), M2(G), mM2, ReZG3 and F (G) are determined. Finally, QSPR-analysis of the above indices with physico-chemical properties of coumarins are presented. The chemical structures of coumarins are depicted in figure 1.

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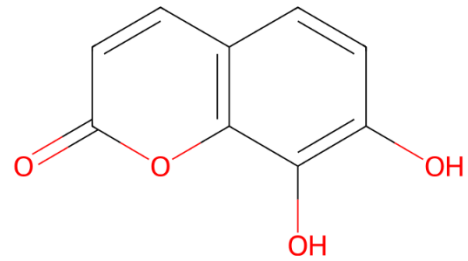
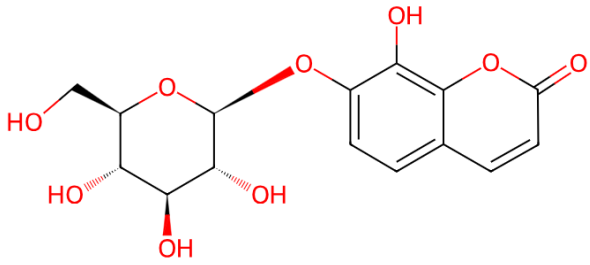
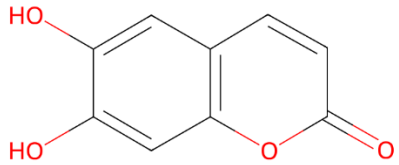
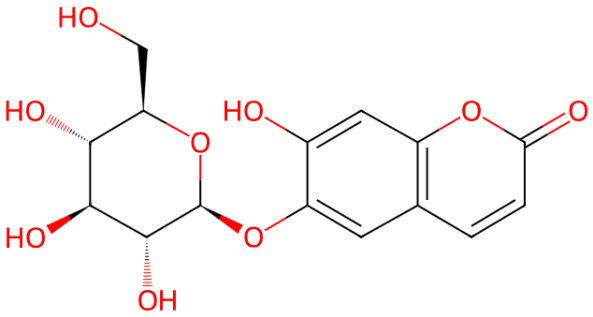
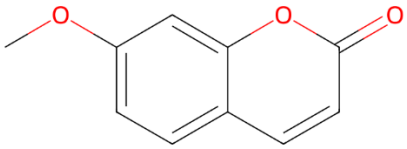
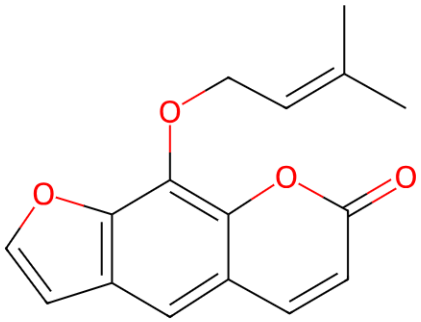
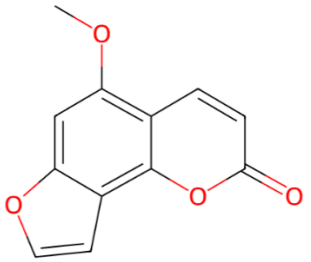
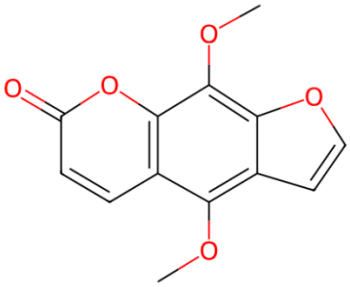
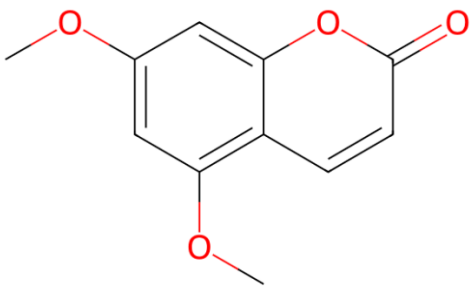
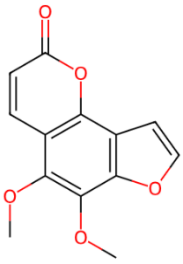

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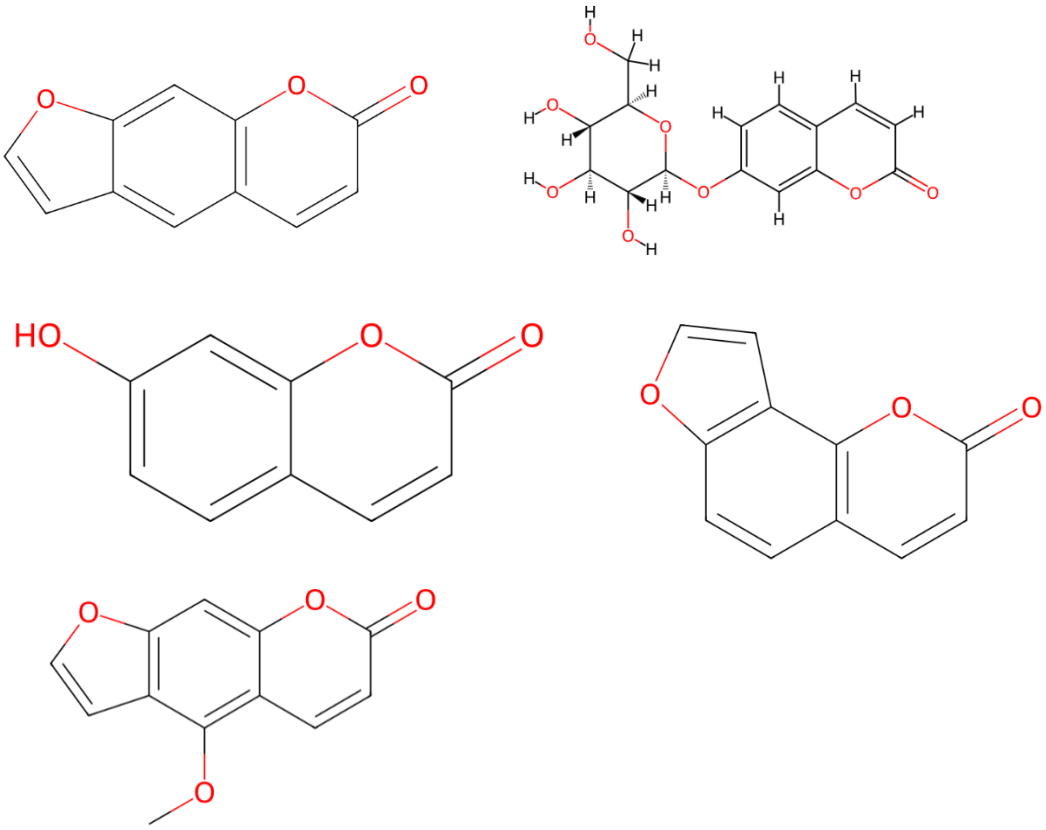

Figure 1. Chemical structures of some simple coumarins.

Graph theory encompasses a wide array of tools, including graph invariants, eigenvalues, polynomials, and more, which are instrumental in various applications. Polynomials, in particular, hold significant importance not only in mathematics but also in fields like medicine. For instance, Hosoya polynomials \cite{12}, Zagreb polynomials, and other similar constructs generate one or more indices. In graph theory, the Hosoya polynomial, introduced by Hosoya, is a distance-based polynomial with numerous chemical applications. It serves as a foundation for deriving all distance-based indices. Subsequently, the Harary polynomial was introduced, also distance-based, from which the Harary index can be derived. Solving a general polynomial typically involves evaluating the polynomial, which may include derivatives, integrals, or both, at a specific point \cite{6a, 8}.

From the Hosoya polynomial, the Wiener index, hyper-Wiener index, and other variants of the Wiener index can be derived. The M-polynomial is a newer concept that serves as a basis for deriving degree-based topological indices. Extensive research is being conducted on the M-polynomial, as it enables the derivation of 11 degree-based topological indices from a single polynomial. Its significance lies in its ability to provide exact forms for most degree-based indices, leading to rapid advancements in this area. Building on the concept of the M-polynomial \cite{45}, the neighborhood degree-based polynomial, known as the NM-polynomial, was introduced \cite{46}. Using the NM-polynomial, 11 neighborhood degree-based topological indices can be derived.

In this study, the M-polynomials are calculated for molecular graphs of coumarins, from which degree-based and neighborhood degree-based topological indices are derived, respectively.

Definition 2.1. \cite{11}
For a simple connected graph G, the M-polynomial is defined as,

$$M(G;x,y) = \sum_{i \leq j} m_{ij}(G) x^i y^j$$

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where m_{ij} represents the number of edges $uv \in E(G)$ such that $\{d(u), d(v)\} = \{i, j\}$. Here $d(u)$, $d(v)$ represent the degrees of the vertices u and v in the graph G.

Table 1. The relation between various TIs with M-polynomial.

Topological index	**Formula** $g(d(u), d(v))$	**Derivation from** $f(x,y) = M(G;x,y)$
M_1	$\sum_{uv \in E(G)} d(u) + d(v)$	$(D_x + D_y)(f(x,y))_{x=1=y}$
M_2	$\sum_{uv \in E(G)} d(u)d(v)$	$(D_x D_y)(f(x,y))_{x=1=y}$
${}^{m}M_2$	$\sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$	$(S_x S_y)(f(x,y))_{x=1=y}$
$ReZG_3$	$\sum_{uv \in E(G)} d(u)d(v)(d(u) + d(v))$	$D_x D_y (D_x + D_y)(f(x,y))_{x=1=y}$
F	$\sum_{uv \in E(G)} d^2(u) + d^2(v)$	$(D_x^2 + D_y^2)(f(x,y))_{x=1=y}$

where $D_x = x\frac{\partial(f(x,y))}{\partial x}$, $D_y = y\frac{\partial(f(x,y))}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t} dt$, $S_y = \int_0^y \frac{f(x,t)}{t} dt$ and $J(f(x,y)) = f(x,x)$.

3. Methodology

In the current work, the molecular structures of coumarins and their derivatives were modeled as molecular graphs. Several degree-based graph invariants were computed. These indices were then numerically compared and presented. Methods such as vertex partitioning, edge partitioning, and combinatorial computations were employed to calculate the aforementioned indices.

Table 2. Edge partitioning of a molecular graph of coumarins.

S. No	Drugs	Edge Partition
1	Daphnetin	$\lvert E_{1,3}\rvert = 3, \lvert E_{2,2}\rvert = 2, \lvert E_{2,3}\rvert = 6, \lvert E_{3,3}\rvert = 3.$
2	Daphnin	$\lvert E_{1,3}\rvert = 6, \lvert E_{2,2}\rvert = 2, \lvert E_{2,3}\rvert = 11, \lvert E_{3,3}\rvert = 6$
3	Esculetin	$\lvert E_{1,3}\rvert = 3, \lvert E_{2,3}\rvert = 9, \lvert E_{3,3}\rvert = 2$
4	Esculin	$\lvert E_{1,2}\rvert = 1, \lvert E_{2,3}\rvert = 14, \lvert E_{1,3}\rvert = 4, \lvert E_{3,3}\rvert = 8$
5	Herniarin	$\lvert E_{1,2}\rvert = 1, \lvert E_{2,2}\rvert = 2, \lvert E_{2,3}\rvert = 13, \lvert E_{1,3}\rvert = 4, \lvert E_{3,3}\rvert = 5$
6	Imperatorin	$\lvert E_{1,2}\rvert = 1, \lvert E_{2,3}\rvert = 9, \lvert E_{1,3}\rvert = 1, \lvert E_{3,3}\rvert = 3$
7	Isobergapten	$\lvert E_{1,3}\rvert = 2, \lvert E_{2,3}\rvert = 8, \lvert E_{3,3}\rvert = 3$
8	Isopimpinellin	$\lvert E_{1,2}\rvert = 2, \lvert E_{1,3}\rvert = 1, \lvert E_{2,3}\rvert = 10, \lvert E_{2,2}\rvert = 1, \lvert E_{3,3}\rvert = 2$
9	Limettin	$\lvert E_{1,3}\rvert = 1, \lvert E_{2,3}\rvert = 8, \lvert E_{2,2}\rvert = 4, \lvert E_{3,3}\rvert = 3$
10	Pimpinellin	$\lvert E_{1,2}\rvert = 1, \lvert E_{1,3}\rvert = 1, \lvert E_{2,3}\rvert = 9, \lvert E_{2,2}\rvert = 3, \lvert E_{3,3}\rvert = 2$
11	Psoralen	$\lvert E_{1,3}\rvert = 3, \lvert E_{2,3}\rvert = 10, \lvert E_{2,2}\rvert = 5, \lvert E_{3,3}\rvert = 4$
12	Skimmin	$\lvert E_{1,2}\rvert = 1, \lvert E_{1,3}\rvert = 1, \lvert E_{2,3}\rvert = 9, \lvert E_{2,2}\rvert = 3, \lvert E_{3,3}\rvert = 4$
13	Umbelliferon	$\lvert E_{1,2}\rvert = 2, \lvert E_{1,3}\rvert = 1, \lvert E_{2,3}\rvert = 8, \lvert E_{2,2}\rvert = 3, \lvert E_{3,3}\rvert = 6$

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14	Angelicin	$\|E_{1,2}\| = 2, \|E_{1,3}\| = 1, \|E_{2,3}\| = 8, \|E_{2,2}\| = 3, \|E_{3,3}\| = 6$
15	Bergapten	$\|E_{1,3}\| = 1, \|E_{2,3}\| = 10, \|E_{2,2}\| = 3, \|E_{3,3}\| = 2$

Details of degrees of end vertices and their edges from Fig. 1 are tabulated in Table 2 for the molecular graph of coumarins. Let $f(x,y) = \mathcal{P}_1$, $D_x f(x,y) = \mathcal{P}_2$, $D_{y} f(x,y) =\mathcal{P}\{3\}$, $(D_x^p D_y^p)(f(x,y))_{x=1=y} = \mathcal{P}_4$, $(S^{p}_{x}S^{p}_{y})(f(x, y))_{x=1=y}=\mathcal{P}\{5\}$, $(D_x S_y + S_x D_y)(f(x,y))_{x=1=y} = \mathcal{P}_6$, $2S_x J(f(x,y))_{x=1} = \mathcal{P}_7$, $S_{x}JD_{x}D_{y}(f(x,y))_{x=1}= \mathcal{P}\{8\}$. The M-polynomials of molecular graphs of coumarins are listed in Table (3)-(6).

Table 3. M-polynomials of molecular graphs of coumarins.

Coumarin	M-polynomial
Daphaetin	$P_1 = 3x^3y^3 + 6x^2y^3 + 2x^2y^2 + 3xy^3$ $P_2 9x^3y^3 + 12x^2y^3 + 4x^2y^2 + 3xy^3$ $P_3 = x^3y^3 + 18x^2y^3 + 4x^2y^2 + 9xy^3$ $P_4 = 18x^3y^3 + 30x^2y^3 + 8x^2y^2 + 12xy^3$ $P_5 = 27x^3y^3 + 36x^2y^3 + 8x^2y^2 + 9xy^3$ $P_6 = 54x^3y^3 + 78x^2y^3 + 16x^2y^2 + 30xy^3$ $P_7 = 3^{2p+1}x^3y^3 + 6^{p+1}x^2y^3 + 2^{2p+1}x^2y^2 + 3^{p+1}xy^3$ $P_8 = 162x^3y^3 + 180x^2y^3 + 32x^2y^2 + 36xy^3$
Daphnin	$P_1 = 6x^3y^3 + 11x^2y^3 + 2x^2y^2 + 6xy^3$ $P_2 = 18x^3y^3 + 22x^2y^3 + 4x^2y^2 + 6xy^3$ $P_3 = 18x^3y^3 + 33x^2y^3 + 4x^2y^2 + 18xy^3$ $P_4 = 36x^3y^3 + 55x^2y^3 + 8x^2y^2 + 24xy^3$ $P_5 = 54x^3y^3 + 66x^2y^3 + 8x^2y^2 + 18xy^3$ $P_6 = 108x^3y^3 + 143x^2y^3 + 16x^2y^2 + 60xy^3$ $P_7 = 2 \cdot 2^{2p}x^2y^2 + 6 \cdot 3^{2p}x^3y^3 + 6 \cdot 3^{p}xy^3 + 11 \cdot 6^{p}x^2y^3$ $P_8 = 324x^3y^3 + 330x^2y^3 + 32x^2y^2 + 72xy^3$
Esculetin	$P_1 = 2x^3y^3 + 9x^2y^3 + 3xy^3$ $P_2 = 6x^3y^3 + 18x^2y^3 + 3xy^3$ $P_3 = 6x^3y^3 + 27x^2y^3 + 9xy^3$ $P_4 = 12x^3y^3 + 45x^2y^3 + 12xy^3$ $P_5 = 18x^3y^3 + 54x^2y^3 + 9xy^3$ $P_6 = 36x^3y^3 + 117x^2y^3 + 30xy^3$ $P_7 = 2 \cdot 3^{2p}x^3y^3 + 3 \cdot 3^{p}xy^3 + 9 \cdot 6^{p}x^2y^3$ $P_8 = 108x^3y^3 + 270x^2y^3 + 36xy^3$

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Table 4. M-polynomials of molecular graphs of coumarins.

Coumarin	M-polynomial
Esculin	$P_1 = 8x^3y^3 + 14x^2y^3 + 4xy^3 + 1xy^2$ $P_2 = 24x^3y^3 + 28x^2y^3 + 4xy^3 + 1xy^2$ $P_3 = 24x^3y^3 + 42x^2y^3 + 12xy^3 + 2xy^2$ $P_4 = 48x^3y^3 + 70x^2y^3 + 16xy^3 + 3xy^2$ $P_5 = 72x^3y^3 + 84x^2y^3 + 12xy^3 + 2xy^2$ $P_6 = 144x^3y^3 + 182x^2y^3 + 40xy^3 + 5xy^2$ $P_7 = 2^p xy^2 + 8 \cdot 3^{2p}x^3y^3 + 4 \cdot 3^p xy^3 + 14 \cdot 6^p x^2y^3$ $P_8 = 432x^3y^3 + 420x^2y^3 + 48xy^3 + 6xy^2$
Skimmin	$P_1 = 5x^3y^3 + 13x^2y^3 + 2x^2y^2 + 4xy^3 + 1xy^2$ $P_2 = 15x^3y^3 + 26x^2y^3 + 4x^2y^2 + 4xy^3 + 1xy^2$ $P_3 = 15x^3y^3 + 39x^2y^3 + 4x^2y^2 + 12xy^3 + 2xy^2$ $P_4 = 30x^3y^3 + 65x^2y^3 + 8x^2y^2 + 16xy^3 + 3xy^2$ $P_5 = 45x^3y^3 + 78x^2y^3 + 8x^2y^2 + 12xy^3 + 2xy^2$ $P_6 = 90x^3y^3 + 169x^2y^3 + 16x^2y^2 + 40xy^3 + 5xy^2$ $P_7 = 2 \cdot 2^{2p}x^2y^2 + 2^p xy^2 + 5 \cdot 3^{2p}x^3y^3 + 4 \cdot 3^p xy^3 + 13 \cdot 6^p x^2y^3$ $P_8 = 270x^3y^3 + 390x^2y^3 + 32x^2y^2 + 48xy^3 + 6xy^2$
Herniarin	$P_1 = 3x^3y^3 + 9x^2y^3 + 1xy^3 + 1xy^2$ $P_2 = 9x^3y^3 + 18x^2y^3 + 1xy^3 + 1xy^2$ $P_3 = 9x^3y^3 + 27x^2y^3 + 3xy^3 + 2xy^2$ $P_4 = 18x^3y^3 + 45x^2y^3 + 4xy^3 + 3xy^2$ $P_5 = 27x^3y^3 + 54x^2y^3 + 3xy^3 + 2xy^2$ $P_6 = 54x^3y^3 + 117x^2y^3 + 10xy^3 + 5xy^2$ $P_7 = 2^p xy^2 + 3 \cdot 3^{2p}x^3y^3 + 3^p xy^3 + 9 \cdot 6^p x^2y^3$ $P_8 = 162x^3y^3 + 270x^2y^3 + 12xy^3 + 6xy^2$
Umbelliferon	$P_1 = 3x^3y^3 + 8x^2y^3 + 2xy^3$ $P_2 = 9x^3y^3 + 16x^2y^3 + 2xy^3$ $P_3 = 9x^3y^3 + 24x^2y^3 + 6xy^3$ $P_4 = 18x^3y^3 + 40x^2y^3 + 8xy^3$ $P_5 = 27x^3y^3 + 48x^2y^3 + 6xy^3$ $P_6 = 54x^3y^3 + 104x^2y^3 + 20xy^3$ $P_7 = 3 \cdot 3^{2p}x^3y^3 + 2 \cdot 3^p xy^3 + 8 \cdot 6^p x^2y^3$ $P_8 = 162x^3y^3 + 240x^2y^3 + 24xy^3$

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Table 5. M-polynomials of molecular graphs of coumarins.

Coumarin	M-polynomial
Limettin	$P_1 = 2x^3y^3 + 10x^2y^3 + 1x^2y^2 + 1xy^3 + 2xy^2$ $P_2 = 6x^3y^3 + 20x^2y^3 + 2x^2y^2 + 1xy^3 + 2xy^2$ $P_3 = 6x^3y^3 + 30x^2y^3 + 2x^2y^2 + 3xy^3 + 4xy^2$ $P_4 = 12x^3y^3 + 50x^2y^3 + 4x^2y^2 + 4xy^3 + 6xy^2$ $P_5 = 18x^3y^3 + 60x^2y^3 + 4x^2y^2 + 3xy^3 + 4xy^2$ $P_6 = 36x^3y^3 + 130x^2y^3 + 8x^2y^2 + 10xy^3 + 10xy^2$ $P_7 = 2^{2p}x^2y^2 + 2 \cdot 2^p xy^2 + 2 \cdot 3^{2p}x^3y^3 + 3^p xy^3 + 10 \cdot 6^p x^2y^3$ $P_8 = 108x^3y^3 + 300x^2y^3 + 16x^2y^2 + 12xy^3 + 12xy^2$
Angelicin	$P_1 = 8x^4y^3 + 3x^3y^3 + 4x^2y^2 + 1xy^3$ $P_2 = 32x^4y^3 + 9x^3y^3 + 8x^2y^2 + 1xy^3$ $P_3 = 24x^4y^3 + 9x^3y^3 + 8x^2y^2 + 3xy^3$ $P_4 = 56x^4y^3 + 18x^3y^3 + 16x^2y^2 + 4xy^3$ $P_5 = 96x^4y^3 + 27x^3y^3 + 16x^2y^2 + 3xy^3$ $P_6 = 200x^4y^3 + 54x^3y^3 + 32x^2y^2 + 10xy^3$ $P_7 = 8 \cdot 12^p x^4y^3 + 4 \cdot 2^{2p}x^2y^2 + 3 \cdot 3^{2p}x^3y^3 + 3^p xy^3$ $P_8 = 672x^4y^3 + 162x^3y^3 + 64x^2y^2 + 12xy^3$
Bergapten	$P_1 = 2x^3y^3 + 9x^2y^3 + 3x^2y^2 + 1xy^3 + 1xy^2$ $P_2 = 6x^3y^3 + 18x^2y^3 + 6x^2y^2 + 1xy^3 + 1xy^2$ $P_3 = 6x^3y^3 + 27x^2y^3 + 6x^2y^2 + 3xy^3 + 2xy^2$ $P_4 = 12x^3y^3 + 45x^2y^3 + 12x^2y^2 + 4xy^3 + 3xy^2$ $P_5 = 18x^3y^3 + 54x^2y^3 + 12x^2y^2 + 3xy^3 + 2xy^2$ $P_6 = 36x^3y^3 + 117x^2y^3 + 24x^2y^2 + 10xy^3 + 5xy^2$ $P_7 = 3 \cdot 2^{2p}x^2y^2 + 2^p xy^2 + 2 \cdot 3^{2p}x^3y^3 + 3^p xy^3 + 9 \cdot 6^p x^2y^3$ $P_8 = 108x^3y^3 + 270x^2y^3 + 48x^2y^2 + 12xy^3 + 6xy^2$
Imperatorin	$P_1 = 4x^3y^3 + 10x^2y^3 + 5x^2y^2 + 3xy^3$ $P_2 = 12x^3y^3 + 20x^2y^3 + 10x^2y^2 + 3xy^3$ $P_3 = 12x^3y^3 + 30x^2y^3 + 10x^2y^2 + 9xy^3$ $P_4 = 24x^3y^3 + 50x^2y^3 + 20x^2y^2 + 12xy^3$ $P_5 = 36x^3y^3 + 60x^2y^3 + 20x^2y^2 + 9xy^3$ $P_6 = 72x^3y^3 + 130x^2y^3 + 40x^2y^2 + 30xy^3$ $P_7 = 5 \cdot 2^{2p}x^2y^2 + 4 \cdot 3^{2p}x^3y^3 + 3 \cdot 3^p xy^3 + 10 \cdot 6^p x^2y^3$ $P_8 = 216x^3y^3 + 300x^2y^3 + 80x^2y^2 + 36xy^3$

https://doi.org/10.71058/jodac.v9i7003

Table 6. M-polynomials of molecular graphs of coumarins.

Coumarin	M-polynomial
Isobergapten	$P_1 = 4x^3y^3 + 9x^2y^3 + 3x^2y^2 + 1xy^3 + 1xy^2$ $P_2 = 12x^3y^3 + 18x^2y^3 + 6x^2y^2 + 1xy^3 + 1xy^2$ $P_3 = 12x^3y^3 + 27x^2y^3 + 6x^2y^2 + 3xy^3 + 2xy^2$ $P_4 = 24x^3y^3 + 45x^2y^3 + 12x^2y^2 + 4xy^3 + 3xy^2$ $P_5 = 36x^3y^3 + 54x^2y^3 + 12x^2y^2 + 3xy^3 + 2xy^2$ $P_6 = 72x^3y^3 + 117x^2y^3 + 24x^2y^2 + 10xy^3 + 5xy^2$ $P_7 = 3 \cdot 2^{2p}x^2y^2 + 2^pxy^2 + 4 \cdot 3^{2p}x^3y^3 + 3^pxy^3 + 9 \cdot 6^px^2y^3$ $P_8 = 216x^3y^3 + 270x^2y^3 + 48x^2y^2 + 12xy^3 + 6xy^2$
Isopimpinellin	$P_1 = 6x^3y^3 + 8x^2y^3 + 3x^2y^2 + 1xy^3 + 2xy^2$ $P_2 = 18x^3y^3 + 16x^2y^3 + 6x^2y^2 + 1xy^3 + 2xy^2$ $P_3 = 18x^3y^3 + 24x^2y^3 + 6x^2y^2 + 3xy^3 + 4xy^2$ $P_4 = 36x^3y^3 + 40x^2y^3 + 12x^2y^2 + 4xy^3 + 6xy^2$ $P_5 = 54x^3y^3 + 48x^2y^3 + 12x^2y^2 + 3xy^3 + 4xy^2$ $P_6 = 108x^3y^3 + 104x^2y^3 + 24x^2y^2 + 10xy^3 + 10xy^2$ $P_7 = 3 \cdot 2^{2p}x^2y^2 + 2 \cdot 2^pxy^2 + 6 \cdot 3^{2p}x^3y^3 + 3^pxy^3 + 8 \cdot 6^px^2y^3$ $P_8 = 324x^3y^3 + 240x^2y^3 + 48x^2y^2 + 12xy^3 + 12xy^2$
Pimpinellin	$P_1 = 6x^3y^3 + 8x^2y^3 + 3x^2y^2 + 1xy^3 + 2xy^2$ $P_2 = 18x^3y^3 + 16x^2y^3 + 6x^2y^2 + 1xy^3 + 2xy^2$ $P_3 = 18x^3y^3 + 24x^2y^3 + 6x^2y^2 + 3xy^3 + 4xy^2$ $P_4 = 36x^3y^3 + 40x^2y^3 + 12x^2y^2 + 4xy^3 + 6xy^2$ $P_5 = 54x^3y^3 + 48x^2y^3 + 12x^2y^2 + 3xy^3 + 4xy^2$ $P_6 = 108x^3y^3 + 104x^2y^3 + 24x^2y^2 + 10xy^3 + 10xy^2$ $P_7 = 3 \cdot 2^{2p}x^2y^2 + 2 \cdot 2^pxy^2 + 6 \cdot 3^{2p}x^3y^3 + 3^pxy^3 + 8 \cdot 6^px^2y^3$ $P_8 = 324x^3y^3 + 240x^2y^3 + 48x^2y^2 + 12xy^3 + 12xy^2$
Psoralen	$P_1 = 2x^3y^3 + 10x^2y^3 + 3x^2y^2 + 1xy^3$ $P_2 = 6x^3y^3 + 20x^2y^3 + 6x^2y^2 + 1xy^3$ $P_3 = 6x^3y^3 + 30x^2y^3 + 6x^2y^2 + 3xy^3$ $P_4 = 12x^3y^3 + 50x^2y^3 + 12x^2y^2 + 4xy^3$ $P_5 = 18x^3y^3 + 60x^2y^3 + 12x^2y^2 + 3xy^3$ $P_6 = 36x^3y^3 + 130x^2y^3 + 24x^2y^2 + 10xy^3$ $P_7 = 3 \cdot 2^{2p}x^2y^2 + 2 \cdot 3^{2p}x^3y^3 + 3^pxy^3 + 10 \cdot 6^px^2y^3$ $P_8 = 108x^3y^3 + 300x^2y^3 + 48x^2y^2 + 12xy^3$

4.1. Three-dimensional plots of the M-polynomials of molecular graphs of coumarins

In this section the three-dimensional plots of the M-polynomial for molecular graphs of coumarins are presented in figures (2)-(4).

https://doi.org/10.71058/jodac.v9i7003

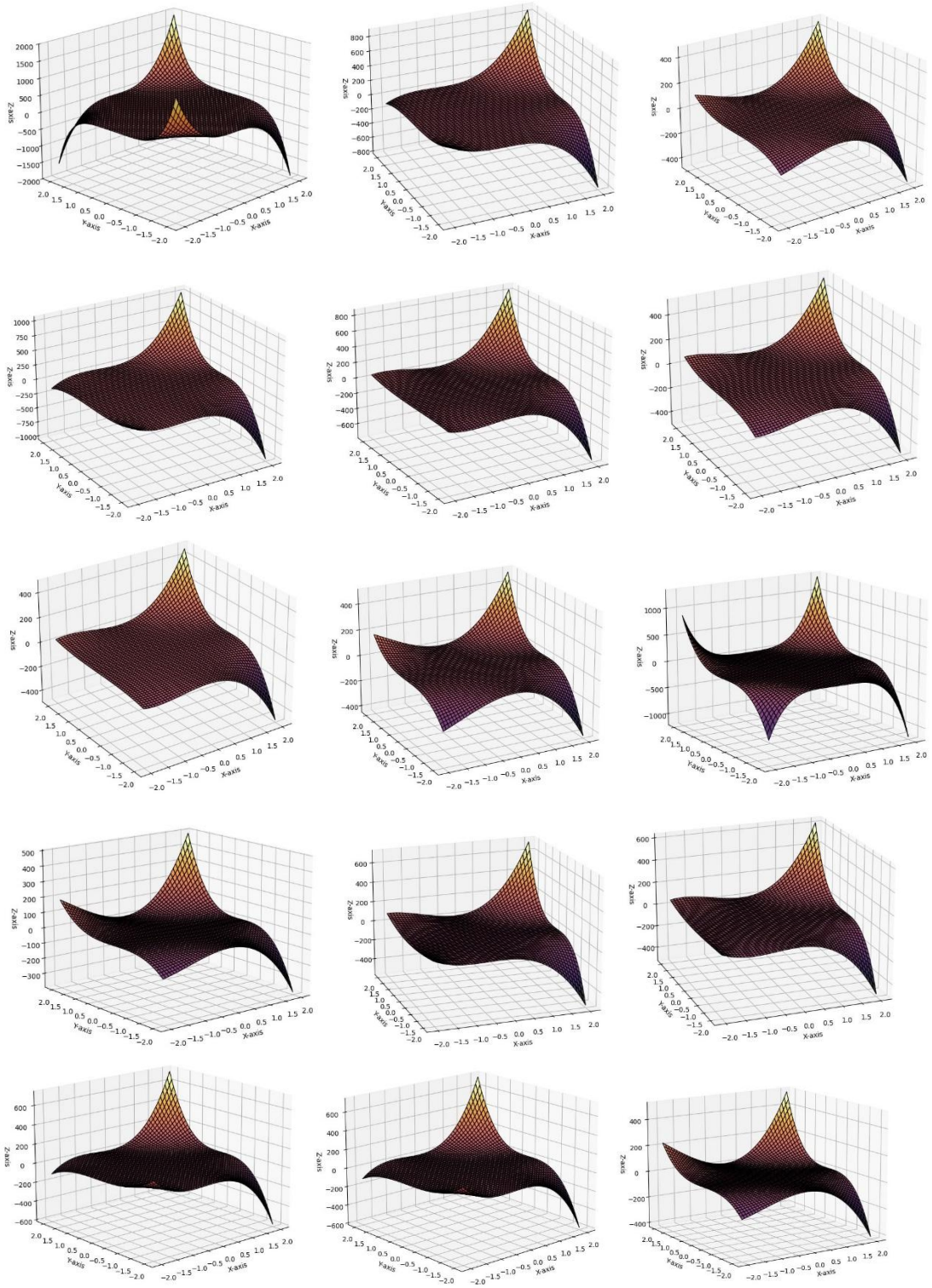

Figure 2. 3D plots of M-polynomials of molecular graphs of coumarins.

https://doi.org/10.71058/jodac.v9i7003

5. QSPR-analysis of M-polynomials with physicochemical properties of coumarins

In [26], studied the QSPR- modeling of coumarins and coumarin-related compounds in pharmacotherapy of cancer using various topological indices. The physical properties of coumarins such as density(D)g/cm^3, boiling point(BP) $^{\circ}C$ at 760 mmHg, vapor pressure(VP) mmHg at $25^{\circ}C$, enthalpy of vaporization(E) kJ/mol, flash point(FP) $^{\circ}C$, index of refraction(IR) cm^3, molar refractivity(MR) A^2, polar surface area(PSA) cm^3, polarizability(P) $dyne/cm$, surface tension(ST) cm^3 and molar volume (MV) were considered for their study. The molecular graphs of coumarins mentioned in Figure 1 can be found in [26].

Table 7. physicochemical properties of coumarins

S. No	Drugs	D	BP	VP	E	FP	IR	MR	PSA	P	ST	MV
1	Daphnetin	1.60	430.40	1.10	71.20	184.50	1.69	43.50	67.00	17.30	75.60	114.00
2	Daphnin	1.70	670.00	2.20	103.40	252.40	1.69	77.40	146.00	30.70	92.60	202.60
3	Esculetin	1.60	469.70	1.20	76.00	201.50	1.69	43.50	67.00	17.30	75.60	114.00
4	Esculin	1.70	697.70	2.30	107.30	262.80	1.69	77.40	146.00	30.70	92.60	202.60
5	Herniarin	1.20	335.30	0.70	57.80	138.60	1.57	46.40	36.00	18.40	44.40	141.10
6	Imperatorin	1.20	448.30	1.10	70.70	224.90	1.61	75.00	49.00	29.70	46.70	217.50
7	Isobergapten	1.40	412.40	1.00	66.50	203.20	1.64	56.60	49.00	22.40	52.00	158.00
8	Isopimpinellin	1.40	448.70	1.10	70.70	225.10	1.61	63.30	58.00	25.10	49.60	182.00
9	Limettin	1.20	388.10	0.90	63.70	176.30	1.56	53.10	45.00	21.10	43.00	165.10
10	Pimpinellin	1.40	441.00	1.10	69.80	220.50	1.61	63.30	58.00	25.10	49.60	182.00
11	Psoralen	1.40	362.60	0.80	60.90	173.10	1.67	49.90	39.00	19.80	55.50	134.00
12	Skimmin	1.60	632.00	1.90	98.20	239.30	1.66	75.50	126.00	29.90	81.40	204.20
13	Umbelliferon	1.40	382.10	0.90	65.50	181.20	1.64	41.60	47.00	16.50	59.50	115.50
14	Angelicin	1.40	362.60	0.80	60.90	173.10	1.67	49.90	39.00	19.80	55.50	134.00
15	Bergapten	1.40	412.40	1.00	66.50	203.20	1.64	56.60	49.00	22.40	52.00	158.00

The topological index values for molecular graphs of coumarins are listed in Table 8 below.

https://doi.org/10.71058/jodac.v9i7003

Table 8. Topological indices for molecular graphs of coumarins

Drugs	M_1	M_2	mM_2	ReZ	F
Daphnetin	68.00	80.00	2.83	410.00	178.00
Daphnin	123.00	146.00	5.00	758.00	327.00
Esculetin	69.00	81.00	2.72	414.00	183.00
Esculin	137.00	170.00	55.00	906.00	371.00
Herniarin	70.00	86.00	2.66	450.00	186.00
Imperatorin	106.00	125.00	4.36	632.00	272.00
Isobergapten	88.00	107.00	3.52	552.00	228.00
Isopimpinellin	98.00	121.00	48.00	636.00	256.00
Limettin	76.00	89.00	3.47	448.00	194.00
Pimpinellin	98.00	121.00	4.08	636.00	256.00
Psoralen	78.00	93.00	2.97	468.00	200.00
Skimmin	122.00	145.00	55.00	746.00	320.00
Umbelliferon	66.00	81.00	2.33	426.00	178.00
Angelicin	94.00	142.00	2.33	910.00	296.00
Bergapten	76.00	89.00	3.30	444.00	192.00

5.1. Regression Models

For QSPR analysis, the following three regression models have been considered for the study:

Linear regression

$$PP = a(TI) + b$$

Quadratic regression

$$PP = a(TI)^2 + b(TI) + c$$

Cubic regression

$$PP = a(TI)^3 + b(TI)^2 + c(TI) + d$$

Where PP denotes the physical property, TI denotes the topological index, and a, b, c are arbitrary constants. We have tested the all three models for the topological indices listed in Table 8 with the physicochemical properties of coumarins(see Table 7). The QSPR models for the various physicochemical properties of coumarin drugs with the best-fitting topological indices are given by:

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Linear Regression for $M_1(G)$:

$$MR = 0.542(M_1(G)) + 8.726$$

$$n = 15 \quad \mathbf{r=0.938} \quad F = 94.395 \; SF = 4.714 \; Sig = 0.000$$

$$P = 0.214(M_1(G)) + 3.507$$

$$n = 15 \quad \mathbf{r=0.938} \quad F = 95.534 \; SF = 1.854 \; Sig = 0.000$$

Quadratic Regression for $M_1(G)$

$$BP = (0.098)(M_1(G))^2 + (-14.987)(M_1(G)) + (965.205)$$

$$n = 15 \quad \mathbf{r=0.930} \quad F = 38.136 \; SF = 45.416 \; Sig = 0.000$$

$$VP = (0.000)(M_1(G))^2 + (-0.075)(M_1(G)) + (3.853)$$

$$n = 15 \quad \mathbf{r=0.937} \quad F = 43.466 \; SF = 0.190 \; Sig = 0.000$$

$$E = (0.015)(M_1(G))^2 + (-2.469)(M_1(G)) + (163.000)$$

$$n = 15 \quad \mathbf{r=0.931} \quad F = 38.838 \; SF = 6.253 \; Sig = 0.000$$

$$MR = (-0.003)(M_1(G))^2 + (1.209)(M_1(G)) + (-22.276)$$

$$n = 15 \quad \mathbf{r=0.945} \quad F = 49.716 \; SF = 4.628 \; Sig = 0.000$$

$$PSA = (0.039)(M_1(G))^2 + (-6.364)(M_1(G)) + (303.437)$$

$$n = 15 \quad \mathbf{r=0.921} \quad F = 33.647 \; SF = 16.076 \; Sig = 0.000$$

$$P = (-0.001)(M_1(G))^2 + (0.473)(M_1(G)) + (-8.533)$$

$$n = 15 \quad \mathbf{r=0.945} \quad F = 50.136 \; SF = 1.823 \; Sig = 0.000$$

Cubic Regression for $M_1(G)$

$$BP = (0.000)(M_1(G))^3 + (32.513)(M_1(G))^2 + (-5.194)M_1(G)) + (649.860)$$

$$n = 15 \quad \mathbf{r=0.925} \quad F = 35.716 \; SF = 46.715 \; Sig = 0.000$$

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$$\text{V P} = (1.545 \times 10^{-6})(\text{M}_1(\text{G}))^3 + (29.716)(\text{M}_1(\text{G}))^2 + (-0.028)\text{M}_1(\text{G})) + (2.334)$$

$$n = 15 \quad \textbf{r=0.933} \quad F = 40.466 \; SF = 0.196 \; Sig = 0.000$$

$$\text{E} = (5.002 \times 10^{-5})(\text{M}_1(\text{G}))^3 + (36.542)(\text{M}_1(\text{G}))^2 + (-0.922)\text{M}_1(\text{G})) + (113.186)$$

$$n = 15 \quad \textbf{r=0.925} \quad F = 35.695 \; SF = 6.485 \; Sig = 0.000$$

$$\text{MR} = (-1.162 \times 10^{-5})(\text{M}_1(\text{G}))^3 + (10.632)(\text{M}_1(\text{G}))^2 + (0.890)\text{M}_1(\text{G})) + (-12.615)$$

$$n = 15 \quad \textbf{r=0.945} \quad F = 50.186 \; SF = 4.609 \; Sig = 0.000$$

$$PSA = (0.000)(M_1(G))^3 + (37.369)(M_1(G))^2 + (-2.445)M_1(G)) + (177.344)$$

$$n = 15 \quad \textbf{r=0.915} \quad F = 31.005 \; SF = 16.640 \; Sig = 0.000$$

$$\text{P} = (-4.516 \times 10^{-6})(\text{M}_1(\text{G}))^3 + (10.663)(\text{M}_1(\text{G}))^2 + (0.350)\text{M}_1(\text{G})) + (-4.786)$$

$$n = 15 \quad \textbf{r=0.946} \quad F = 50.605 \; SF = 1.815 \; Sig = 0.000$$

Cubic Regression for ${}^{m}M_2(G)$

$$MR = (0.006)({}^{m}M_2(G))^3 + (-0.656)({}^{m}M_2(G))^2 + (17.806){}^{m}M_2(G)) + (3.288)$$

$$n = 15 \quad \textbf{r=0.962} \quad F = 45.279 \; SF = 4.032 \; Sig = 0.000$$

$$P = (0.003)({}^{m}M_2(G))^3 + (-0.259)({}^{m}M_2(G))^2 + (7.042){}^{m}M_2(G)) + (1.362)$$

$$n = 15 \quad \textbf{r=0.962} \quad F = 45.952 \; SF = 1.583 \; Sig = 0.000$$

$$MV = (0.017)({}^{m}M_2(G))^3 + (-1.790)({}^{m}M_2(G))^2 + (49.719){}^{m}M_2(G)) + (8.905)$$

$$n = 15 \quad \textbf{r=0.938} \quad F = 26.990 \; SF = 13.901 \; Sig = 0.000$$

Scatter plots with best fit lines for above mentioned regression models are shown in the following figures:

https://doi.org/10.71058/jodac.v9i7003

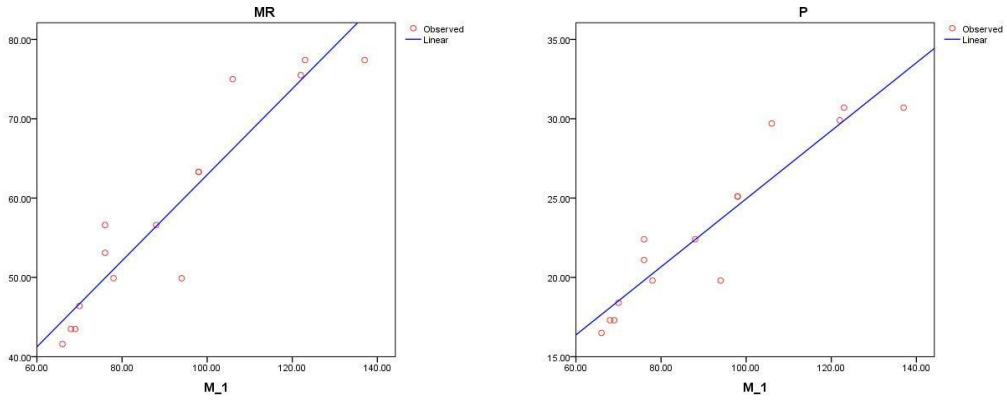

Figure 5. Linear regression model of MR and P with $M_1(G)$

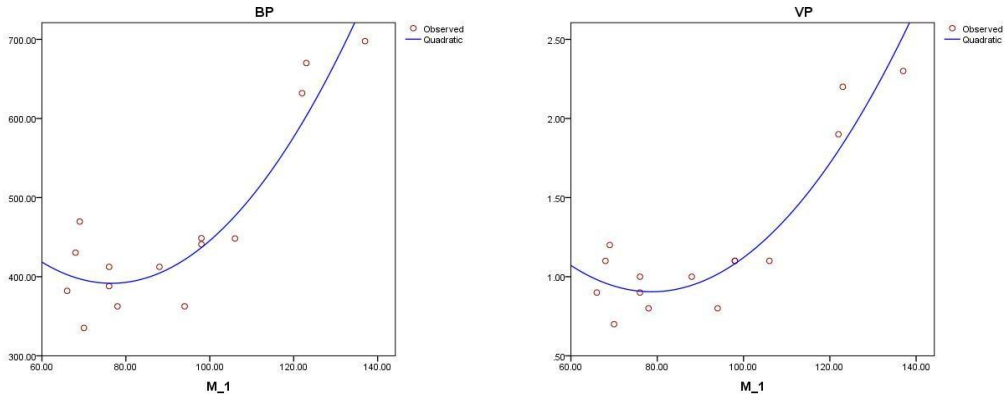

Figure 6. Quadratic regression model of BP and VP with $M_1(G)$

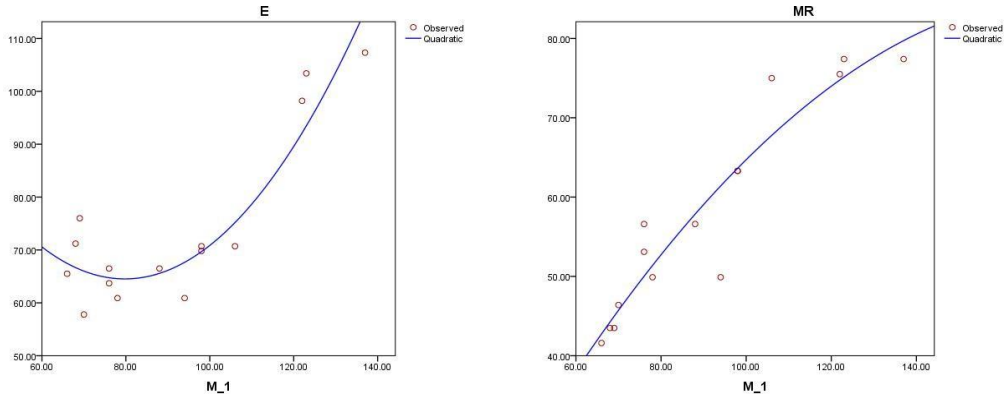

Figure 7. Quadratic regression model of E and MR with $M_1(G)$

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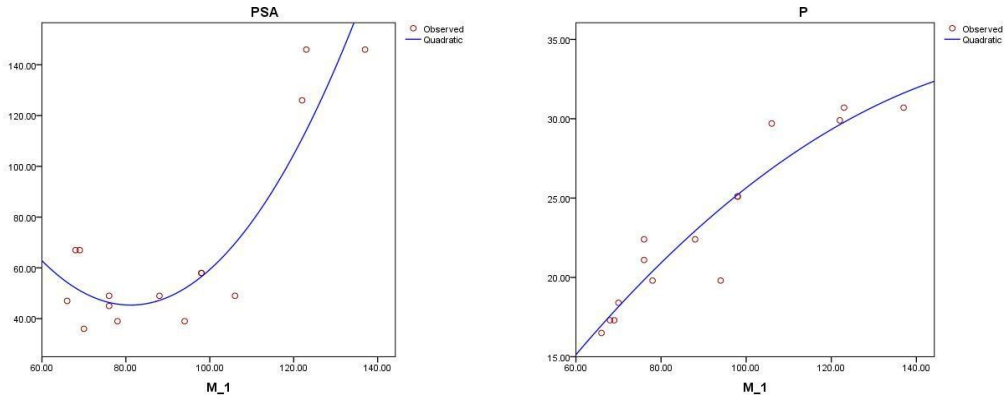

Figure 8. Quadratic regression model of PSA and P with $M_1(G)$

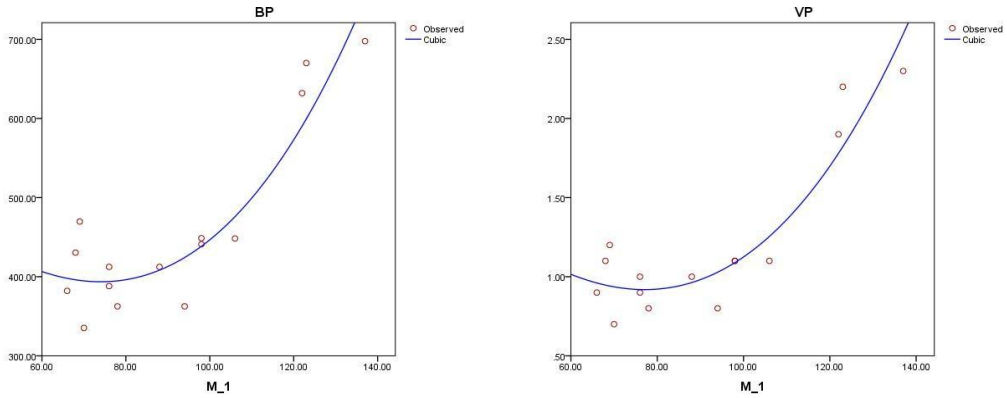

Figure 9. Cubic regression model of BP and VP with $M_1(G)$

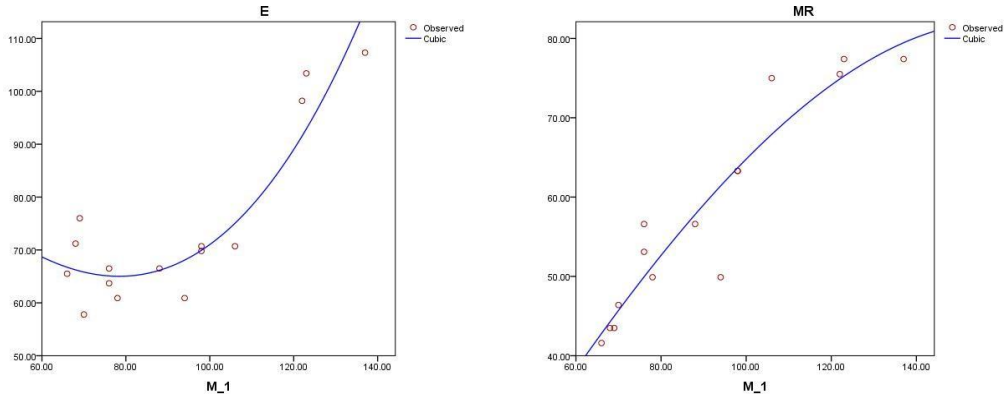

Figure 10. Cubic regression model of E and MR with $M_1(G)$

https://doi.org/10.71058/jodac.v9i7003

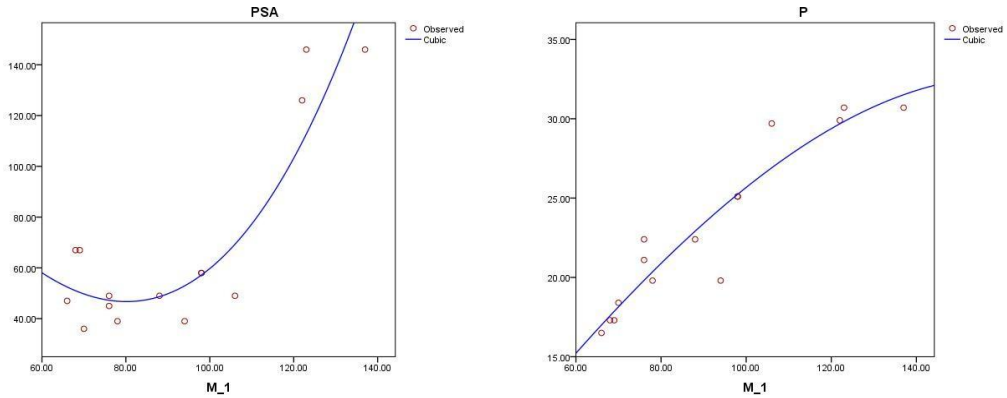

Figure 11. Cubic regression model of PSA and P with $M_1(G)$

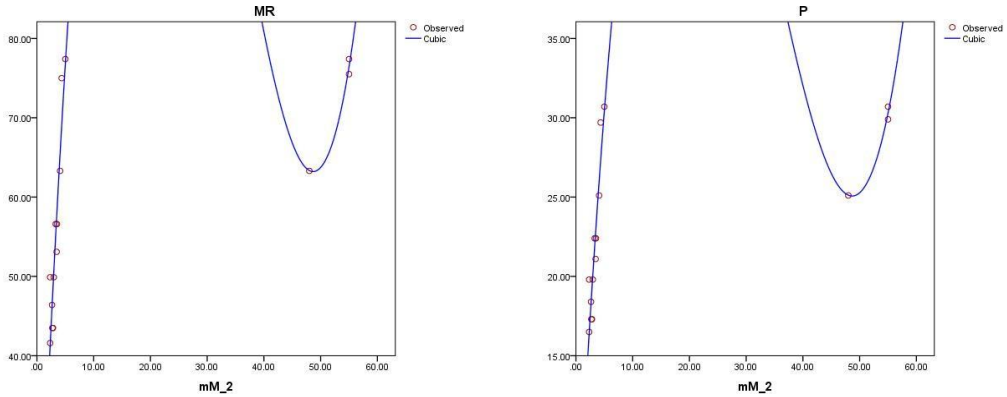

Figure 12. Cubic regression model of MR and P with ${}^{m}M_2(G)$

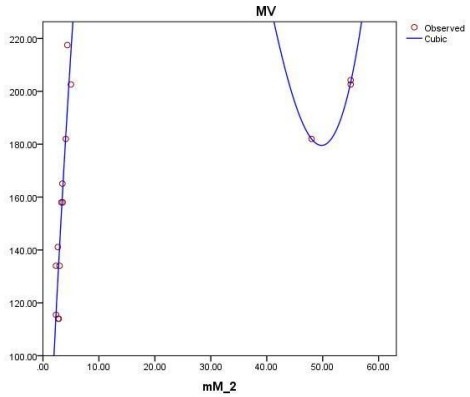

Figure 13. Cubic regression model of MV with ${}^{m}M_2(G)$

1.1 Statistical Analysis of QSPR Models

In a regression model, different parameters serve distinct purposes. The significance of the data is determined by the p-value, a key statistic in regression analysis. The p-value helps evaluate the importance of each predictor in the model by indicating the probability that the observed

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relationship between the dependent variable and the predictor occurred by chance. A low p- value, typically below 0.05, suggests that the predictor has a statistically significant impact on the dependent variable, providing strong evidence that it contributes meaningfully to the model. Conversely, a high p-value implies that the predictor is not statistically significant and may not explain much of the variance in the dependent variable. The constant in the model is denoted by A, while the coefficient is represented by B. The correlation coefficient, r, measures the relationship between the calculated and experimental values of the physical attributes. The value of r can be either negative (indicating an inverse relationship) or positive (indicating a direct relationship).

Basically, 5 degree based topological indices namely the first Zagreb index $M_1(G)$, the second Zagreb index $M_2(G)$, the second-order modified Zagreb index ${}^{m}M_2(G)$, the redefined third Zagreb index $ReZG_3$ and the forgotten index $F(G)$ were considered for the study(see Table 8) with respect to 11 physicochemical properties of coumarins(see Table 7). Among three regression models we have noticed the following observations:

For *linear regression model*, the first Zagreb index $M_1(G)$ is the only topological index which shows high predicting power among molar refraction and polarizability of coumarins with correlation coefficient **r=0.938** respectively. Further, in both cases, $p = 0.0000$ implies that the linear regression model with respect to MR and P are highly significant.

For *quadratic regression model* again the first Zagreb index $M_1(G)$ is the is the only topological index which shows high predicting power among BP, VP, E, MR, PSA and P with correlation coefficient values ranging from **0.921 to 0.945**. In all the cases, $p = 0.0000$ implies that the quadratic regression model with respect to $M_1(G)$ highly significant.

For *cubic regression model*, the first Zagreb index $M_1(G)$ and the second-order modified Zagreb index ${}^{m}M_2(G)$ shows high predicting power among BP, VP, E, MR, PSA, P and MR, P, MV respectively with correlation coefficient values ranging from **0.915 to 0.962**. In all the cases, $p = 0.0000$ implies that the quadratic regression models with respect to $M_1(G)$ and ${}^{m}M_2(G)$ are highly significant.

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Conclusion

Coumarins exhibit a wide range of biological activities, such as disease prevention, growth modu- lation, and antioxidant properties. Scientific studies have demonstrated that these compounds possess antitumor effects, which are attributed to their influence on immune regulation, cell growth, and differentiation. In the present work, various degree-based topological indices are computed using M-polynomial for molecular graphs of coumarins. A 3D-plots of M-polynomial for molecular graphs of coumarins are presented in figures (2)-(4). Further, the QSPR analysis revealed that the first Zagreb index is the potential topological index to predict physicochemical properties of coumarins.

References

[1] Abdul Rauf, Muhammad Naeem, Adnan Aslam, Quantitative structure–property rela- tionship of edge weighted and degree-based entropy of benzene derivatives, Int. J. Quant. Chem. 122 (2021), e26839.

[2] A.T. Balaban, J. Devillers, Topological Indices and Related Descriptors in QSAR and QSPR, CRC Press, London, 2014.

[3] A. Q. Baig, M. Imran, H. Ali, Computing omega, sadhana and PI polynomials of benzenoid carbon nanotubes, Optoelectronics and advanced materials-rapid communications, vol. 9, 2015, pp. 248–255.

[4] B. Basavanagoud, A.P. Barangi, M-polynomial of some cactus chains and their topological indices, Open Journal of Discrete Applied Mathematics, vol. 2, 2019, pp. 59–67.

[5] D. Bonchev, Information Theoretic Indices for Characterization of Chemical Structures, Research Studies Press, 1983.

[6] Bruneton, J. Immunotoxicity of Epicutaneously Applied Anti-Coagulant Rodenticide War- farin; Intercept Ltd.: Hampshire, UK, 1999; pp. 245–263.

[7] Bruneton, J. Pharmacognosy, Phytochemistry, Medicinal Plants, 2nd ed.; Intercept Ltd.: Hampshire, UK, 1999; pp. 263–277.

[8] J.C. Dearden, Advances in QSAR Modeling, Springer, Cham, Switzerland, 2017, pp. 57–58.

[9] E. Deutsch, S. Klavzar, M-polynomial and Degre Based topological indices, Iranian Journal of Mathematical Chemistry 6 (2015) 93–102.

[10] E. Estrada E, E. Uriarte, Recent advances on the role of topological indices in drug dis- covery research, Curr. Med. Chem. 8 (13) (2001) 1573–1588.

[11] I. Gutman, Some properties of the wiener polynomials, Graph

https://doi.org/10.71058/jodac.v9i7003

Theory Notes, vol. 125, 1993, pp. 13–18 (New York, USA).

[12] F. Harary, Graph Theory, Addison-Wesely, Reading Mass, 1969.

[13] Harishchandra S. Ramane, Raju B. Jummannaver, Note on forgotten topological index of chemical structure in drugs, Applied Mathematics and Nonlinear Sciences 1 (2016) 369–374.

[14] H. Hosoya, On some counting polynomials in chemistry, Discrete Appl. Math., vol. 19, 1988, pp. 239–257.

[15] Lacy, A.; O'Kennedy, R. Studies on coumarins and coumarin–related compounds to de- termine their therapeutic role in the treatment of cancer. Curr. Pharm. Des. 2004, 10, 3797–3811.

[16] Mohammad Reza Farahani, Computing edge-PI index and vertex-PI index of circum- coronene series of benzenoid hk by use of cut method, International Journal of Mathe- matical and Applied Computing 1 (2013) 41–50.

[17] S. Mondal, M. Kamran, N. De, A. Pal, Topological properties of para-line graph of some convex polytopes using neighborhood M-polynomial, Biointerface Research in Applied Chemistry 11 (2021) 9915–9927.

[18] Muhammad Nadeem, Awais Yousaf, Abdul Razaq, Certain Polynomials and Related Topo- logical Indices for the Series of Benzenoid Graphs, Scientific Reports, 2019, pp. 1–6.

[19] S. Nikolic, N. Trinajstic, The Wiener index: development and applications, Croat.Chem. Acta 68 (1) (1995 Feb 1) 105–129.

[20] Ojala, T. Biological Screening of Plant Coumarins. Ph.D. Thesis, University of Helsinki, Helsinki, Finland, 2001.

[21] M.C. Shanmukha, A. Usha, K.C. Shilpa, N.S. Basavarajappa, M-polynomial and neigh- borhood M-polynomial methods for topological indices of porous graphene, The European Physical Journal Plus, vol. 136, No. 10, 2021, pp. 1–6.

[22] M. Randic, Novel molecular descriptor for structure-property studies, Chem. Phys. Lett. 211 (1993) 478–483.

[23] Syed Ajaz K. Kirmani, Parvez Ali, Faizul Azam, Topological indices and QSPR/QSAR analysis of some antiviral drugs being investigated for the treatment of COVID-19 patients, Int. J. Quant. Chem. (2021) 1–22.

[24] Sourav Mondal, Muhammad Imran, Nilanjan De, Anita Pal, Neighborhood Mpolynomial of titanium compounds, Arab. J. Chem., vol. 14, 2021, 103244.

[25] M.C. Shanmukha, N.S. Basavarajappa, A. Usha, K.C. Shilpa, Novel neighborhood re- defined first and second Zagreb indices on carborundum structures, Journal of Applied Mathematics and Computing (2020) 1–14,

[26] Timmanaikar, S.T., Hayat, S., Hosamani, S.M. et al. Structure–property modeling of coumarins and coumarin-related compounds in pharmacotherapy of cancer by employing graphical topological indices. Eur. Phys. J. E, vol. 47, No. 31, 2024.

[27] R. Todeschini, V. Consonni, Handbook of Molecular

https://doi.org/10.71058/jodac.v9i7003

Descriptors, Wiley-VCH, Weinheim, 2000.

[28] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.

[29] A. Usha, M.C. Shanmukha, K.C. Shilpa, B.M. Praveen, Comparative study of degree- based molecular descriptors of cyclodextrins through M-polynomial and NM-polynomial, Journal of the Indian Chemical Society, vol. 100, 2023, 100999.

[30] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.

[31] C.C. Wei, H. Ali, M.A. Binyamin, M.N. Naeem, J.-B. Liu, Computing degree-based topo- logical properties of third type of hex-derived networks, Mathematics 7 (2019) 368.

[32] Weidong Zhao, M.C. Shanmukha, A. Usha, Mohammad reza farahani and K.C. Shilpa, computing SS index of certain dendrimers, J. Math. 2021 (2021), 7483508

[33] Yuede Ma, Matthias Dehmer, Urs-Martin Künzi, Shailesh Tripathi, Modjtaba Ghorbani, Tao Jin, Frank Emmert-Streib, The usefulness of topological indices, Inf. Sci. 606 (2022) 143–151.

[34] A. Yurtas, M. Togan, V. Lokesha, et al., Inverse problem for Zagreb indices, J. Math. Chem. 57 (2019) 609–615.

[35] Zahid Iqbal, Adnan Aslam, Muhammad Ishaq, Wei Gao, On computations of topological descriptors of kagome lattice, Polycycl. Aromat. Comp. (2021) 1–15.