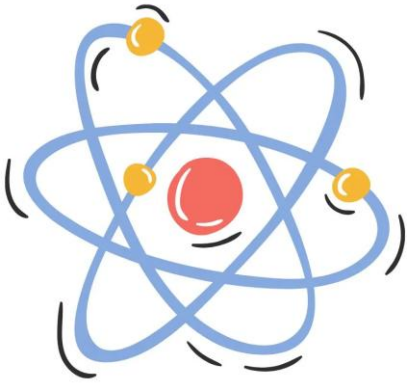

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Rahul Munavalli[1], Prashant Patil[2], Sunilkumar M. Hosamani[3]

[1]Department of Mathematics, Vidyavardhaka College of Engineering, Mysore– 570 002, India and Visvesvaraya Technological University, Belagavi–590018, Karnataka, India.

[2]Department of Mathematics, Jain College of Engineering, Belagavi-590014, India and Visvesvaraya Technological University, Belagavi-590018, Karnataka, India.

[3]Department of Mathematics, Rani Channamma University, Belagavi - 591156, Karnataka, India

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Rahul Munavalli[1], Prashant Patil[2], Sunilkumar M. Hosamani[3]

[1]Department of Mathematics, Vidyavardhaka College of Engineering, Mysore− 570 002, India and Visvesvaraya Technological University, Belagavi−590018, Karnataka, India.
[2]Department of Mathematics, Jain College of Engineering, Belagavi- 590014, India and Visvesvaraya Technological University, Belagavi-590018, Karnataka, India.
[3]Department of Mathematics, Rani Channamma University, Belagavi - 591156, Karnataka, India

[1]rahul1008.mm@gmail.com, [2]prashant66.sdm@gmail.com, 3sunilkumar.rcu@gmail.com

Abstract: *The study of chemical and physical properties of drugs used to treat various types of cancer, based on their molecular structures, has garnered considerable interest, especially through the application of topological indices derived from these structures. A thorough understanding of these properties is essential for drug development. In this context, topological indices play a vital role in connecting chemistry with the pharmaceutical industry by offering an economical method to assess the physical properties of molecules. This study focuses on analyzing the topological polynomials and indices of a series of drugs based on polyphenolic compounds such as coumarins in the treatment of cancer. A set of 05 degree based topological indices are considered viz. generalized Randić index* $\mathbf{R_p(G)}$*, generalized reciprocal Randić index* $\mathbf{RR_p(G)}$*, symmetric division degree index* $\boldsymbol{SDD(G)}$*, harmonic index* $\mathbf{H(G)}$ *and inverse sum index* $\mathbf{I(G)}$ *for this study. Further, A QSPR analysis has been performed to establish the mathematical relationship between the chemical and physical properties of drugs—such as exact mass, molecular weight, heavy atom count, complexity, molar refractivity, and polarizability—and their topological indices. The topological indices used for the drugs in this study demonstrate a strong correlation with their physicochemical properties of coumarins.*

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

1. Introduction

Cancer remains one of the leading causes of disease-related mortality worldwide. Despite the development of numerous chemotherapeutic agents designed to target uncontrolled cell proliferation in various cancers, their application is often associated with significant side effects. Furthermore, the rise of multi-drug resistance presents a major obstacle in the effective treatment of cancer. Common symptoms of cancer include the development of tumors, abnormal bleeding, persistent coughing, unexplained weight loss, and other signs. Major risk factors for cancer include tobacco use, obesity, unhealthy dietary patterns, lack of physical activity, and excessive alcohol consumption. Treatment options for cancer encompass surgery, radiation therapy, chemotherapy, hormone therapy, targeted therapy, and other modalities. Among these, anticancer drugs, including alkylating agents and metabolic modulators, play a vital role in the management of the disease.

Coumarins are polyphenolic compounds characterized as colorless, crystalline oxygenated heterocyclic molecules. They were first identified by Vogel in 1820 when he isolated them from the Fabaceae plant Dipteryx odorata Willd, commonly known as "coumaroun" [6, 7]. Oxygenated heterocyclic compounds encompass furan derivatives, which consist of 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].

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Chemical graphs provide a non-numerical depiction of chemical structures and are extensively utilized in computing structural descriptors for QSAR/QSPR modeling [22, 30]. In this representation, chemical compounds are modeled as graphs, with atoms depicted as vertices and their bonds as edges. Hydrogen atoms are usually excluded in chemical graphs. Topological indices have been shown to encapsulate significant information about the three-dimensional structural characteristics of compounds [1, 16].

Chemistry provides a foundational basis for the application of graph theory in diverse scientific disciplines. Graphical invariants, also referred to as topological indices, are essential tools that supply valuable information, aiding chemists in advancing their research. These invariants predict various molecular properties of a compound by analyzing and characterizing the topological structure of the molecule's graph representation [27, 28].

Topological graph measures are crucial for quantitatively describing graphs. These measures can be categorized into two primary types: information-theoretic and non-information-theoretic. They can also be subdivided into graph invariants based on vertex degrees, distances, eigenvalues, and other attributes. Additionally, they are classified into symmetry measures, cyclicity measures, and branching measures. A wide array of topological graph measures has been developed and is extensively utilized in various fields, including mathematical chemistry, bioinformatics, computer science, and others [33].

In recent years, significant advancements have been achieved in QSAR/QSPR modeling through the use of topological descriptors [2, 5, 8, 25, 32]. The integration of topological indices with hydrophobicity has facilitated the establishment of QSAR/QSPR relationships. Topological descriptors are employed to distinguish between drug and non-drug compounds [10,13]. These indices are vital for identifying numerous compounds in combinatorial syntheses and enabling rapid toxicity screening. Their widespread adoption is due to their cost-efficiency in designing effective drugs while reducing the risks associated with new chemicals. Topological indices (TIs) have gained prominence because they allow for quick computation and extraction of extensive molecular structure information without requiring experimental procedures [31, 34, 35].

Modifications in the chemical structure of organic compounds result in systematic changes in their physicochemical properties and biological properties. Computational chemists aim to establish quantitative relationships between structural features and properties to facilitate diagnostic and mechanistic interpretation or activity prediction [23]. Topological indices help chemists decide whether a chemical compound should be incorporated into a drug formulation by evaluating its index range. Each index has a defined range, and if a compound exceeds the upper limit of this range, it is typically deemed unsuitable for inclusion in drug formulations intended for use by living organisms.

Topological indices are highly useful in QSPR studies, as they establish correlations between physical properties and molecular structures. Wiener pioneered the use of the Wiener index in structure-property studies, finding that it closely aligned with the boiling points of alkanes [19]. Since then, numerous studies have employed this index to link the physical and chemical properties of compounds, greatly 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 graph. 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 $R_p(G)$, $RR_p(G)$, $SDD(G)$, $H(G)$ and $I(G)$ 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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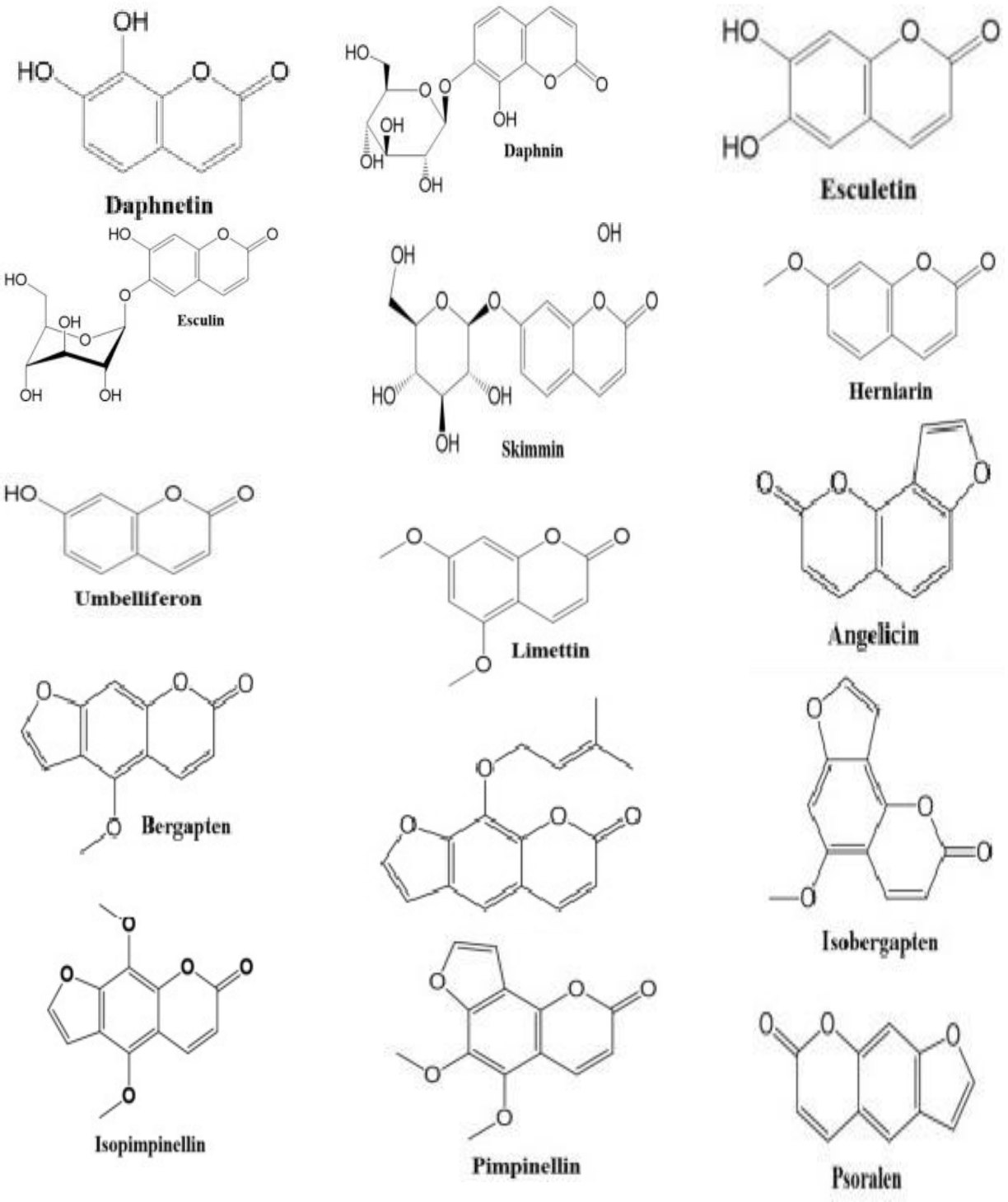

Figure 1: Chemical structures of some simple coumarins.

2. M-Polynomials

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 [33],

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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 [1, 22].

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 [9], the neighborhood degree-based polynomial, known as the NM-polynomial, was introduced [17]. 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 topological indices are derived, respectively.

Definition 2.1. [29] For a simple connected graph G, the M-polynomial is defined as,

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

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** $f(x,y) = M(G;x,y)$
R_p	$\sum_{uv\in E(G)}\{d(u)d(v)\}^p$	$(D_x^p D_y^p)(f(x,y))_{x=1=y}$
RR_p	$\sum_{uv\in E(G)} \frac{1}{d(u)d(v)^p}$	$(S_x^p S_y^p)(f(x,y))_{x=1=y}$
SDD	$\sum_{uv\in E(G)} \frac{d^2(u)+d^2(v)}{d(u)d(v)}$	$(D_x S_y + S_x D_y)(f(x,y))_{x=1=y}$
H	$\sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$	$2S_x J(f(x,y))_{x=1}$
I	$\sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$	$S_x J D_x D_y (f(x,y))_{x=1}$

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.

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

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

4. Results for M-Polynomials

Details of degrees of end vertices and their edges from Fig. 1 are tabulated in Table 2 for the molecular graph of coumarins. Let $f(x,y) = \mathcal{P}_1$, $D_x f(x,y) = \mathcal{P}_2$, $D_y f(x,y) = \mathcal{P}_3$, $(D_x^p D_y^p)(f(x,y))_{x=1=y} = \mathcal{P}_4$, $(S_x^p S_y^p)(f(x,y))_{x=1=y} = \mathcal{P}_5$, $(D_x S_y + S_x D_y)(f(x,y))_{x=1=y} = \mathcal{P}_6$, $2S_x J(f(x,y))_{x=1} = \mathcal{P}_7$, $S_x J D_x D_y (f(x,y))_{x=1} = \mathcal{P}_8$, The M-polynomials of molecular graphs of coumarins are listed in Table (3)-(6).

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

Coumarin	M-polynomial
Daphaetin	$\mathcal{P}_1 = 3x^3y^3 + 6x^2y^3 + 2x^2y^2 + 3xy^3$ $\mathcal{P}_2 = 9x^3y^3 + 12x^2y^3 + 4x^2y^2 + 3xy^3$ $\mathcal{P}_3 = 9x^3y^3 + 18x^2y^3 + 4x^2y^2 + 9xy^3$ $\mathcal{P}_4 = 3^{2p+1}x^3y^3 + 6^{p+1}x^2y^3 + 2^{2p+1}x^2y^2 + 3^{p+1}xy^3$ $\mathcal{P}_5 = 3^{1-2p}x^3y^3 + 6^{1-p}x^2y^3 + 2^{1-2p}x^2y^2 + 3^{1-p}xy^3$ $\mathcal{P}_6 = 6x^3y^3 + 13x^2y^3 + 4x^2y^2 + 10xy^3$ $\mathcal{P}_7 = 1x^3y^3 + 2.4x^2y^3 + 1x^2y^2 + 1.5xy^3$ $\mathcal{P}_8 = 4.5x^3y^3 + 7.2x^2y^3 + 2x^2y^2 + 2.25xy^3$
Daphnin	$\mathcal{P}_1 = 6x^3y^3 + 11x^2y^3 + 2x^2y^2 + 6xy^3$ $\mathcal{P}_2 = 18x^3y^3 + 22x^2y^3 + 4x^2y^2 + 6xy^3$ $\mathcal{P}_3 = 18x^3y^3 + 33x^2y^3 + 4x^2y^2 + 18xy^3$ $\mathcal{P}_4 = 2 \cdot 2^{2p}x^2y^2 + 6 \cdot 3^{2p}x^3y^3 + 6 \cdot 3^{p}xy^3 + 11 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 16^{-p}x^2y^3 + 6 \cdot 3^{-p}xy^3 + 6 \cdot 3^{-2p}x^3y^3 + 2 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 12x^3y^3 + 23.83x^2y^3 + 4x^2y^2 + 20xy^3$ $\mathcal{P}_7 = 2x^3y^3 + 4.4x^2y^3 + 1x^2y^2 + 3xy^3$ $\mathcal{P}_8 = 9x^3y^3 + 13.2x^2y^3 + 2x^2y^2 + 4.5xy^3$
Esculetin	$\mathcal{P}_1 = 2x^3y^3 + 9x^2y^3 + 3xy^3$ $\mathcal{P}_2 = 6x^3y^3 + 18x^2y^3 + 3xy^3$ $\mathcal{P}_3 = 6x^3y^3 + 27x^2y^3 + 9xy^3$ $\mathcal{P}_4 = 2 \cdot 3^{2p}x^3y^3 + 3 \cdot 3^{p}xy^3 + 9 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 9 \cdot 6^{-p}x^2y^3 + 3 \cdot 3^{-p}xy^3 + 2 \cdot 3^{-2p}x^3y^3$ $\mathcal{P}_6 = 4x^3y^3 + 19.5x^2y^3 + 10xy^3$ $\mathcal{P}_7 = 0.66x^3y^3 + 3.6x^2y^3 + 1.5xy^3$ $\mathcal{P}_8 = 3x^3y^3 + 10.8x^2y^3 + 2.25xy^3$

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

Coumarin	M-polynomial
Esculin	$\mathcal{P}_1 = 8x^3y^3 + 14x^2y^3 + 4xy^3 + 1xy^2$ $\mathcal{P}_2 = 24x^3y^3 + 28x^2y^3 + 4xy^3 + 1xy^2$ $\mathcal{P}_3 = 24x^3y^3 + 42x^2y^3 + 12xy^3 + 2xy^2$ $\mathcal{P}_4 = 2^p xy^2 + 8 \cdot 3^{2p} x^3y^3 + 4 \cdot 3^p xy^3 + 14 \cdot 6^p x^2y^3$ $\mathcal{P}_5 = 14 \cdot 6^{-p} x^2y^3 + 4 \cdot 3^{-p} xy^3 + 8 \cdot 3^{-2p} x^3y^3 + 2^{-p} xy^2$ $\mathcal{P}_6 = 16x^3y^3 + 30.33x^2y^3 + 13.33xy^3 + 2.5xy^2$ $\mathcal{P}_7 = 2.66x^3y^3 + 5.6x^2y^3 + 2xy^3 + 0.66xy^2$ $\mathcal{P}_8 = 12x^3y^3 + 16.8x^2y^3 + 3xy^3 + 0.66xy^2$
Herniarin	$\mathcal{P}_1 = 5x^3y^3 + 13x^2y^3 + 2x^2y^2 + 4xy^3 + 1xy^2$ $\mathcal{P}_2 = 15x^3y^3 + 26x^2y^3 + 4x^2y^2 + 4xy^3 + 1xy^2$ $\mathcal{P}_3 = 15x^3y^3 + 39x^2y^3 + 4x^2y^2 + 12xy^3 + 2xy^2$ $\mathcal{P}_4 = 2 \cdot 2^{2p} x^2y^2 + 2^p xy^2 + 5 \cdot 3^{2p} x^3y^3 + 4 \cdot 3^p xy^3 + 13 \cdot 6^p x^2y^3$ $\mathcal{P}_5 = 13 \cdot 6^{-p} x^2y^3 + 4 \cdot 3^{-p} xy^3 + 5 \cdot 3^{-2p} x^3y^3 + 2^{-p} xy^2 + 2 \cdot 2^{-2p} x^2y^2$ $\mathcal{P}_6 = 10x^3y^3 + 28.16x^2y^3 + 4x^2y^2 + 13.33xy^3 + 2.5xy^2$ $\mathcal{P}_7 = 1.66x^3y^3 + 5.2x^2y^3 + 1x^2y^2 + 2xy^3 + 0.66xy^2$ $\mathcal{P}_8 = 7.5x^3y^3 + 15.6x^2y^3 + 2x^2y^2 + 3xy^3 + 0.66xy^2$
Imperatorin	$\mathcal{P}_1 = 3x^3y^3 + 9x^2y^3 + 1xy^3 + 1xy^2$ $\mathcal{P}_2 = 9x^3y^3 + 18x^2y^3 + 1xy^3 + 1xy^2$ $\mathcal{P}_3 = 9x^3y^3 + 27x^2y^3 + 3xy^3 + 2xy^2$ $\mathcal{P}_4 = 162x^3y^3 + 270x^2y^3 + 12xy^3 + 6xy^2$ $\mathcal{P}_5 = 9 \cdot 6^{-p} x^2y^3 + 3^{-p} xy^3 + 3 \cdot 3^{-2p} x^3y^3 + 2^{-p} xy^2$ $\mathcal{P}_6 = 6x^3y^3 + 19.5x^2y^3 + 3.33xy^3 + 2.5xy^2$ $\mathcal{P}_7 = 1x^3y^3 + 3.6x^2y^3 + 0.5xy^3 + 0.66xy^2$ $\mathcal{P}_8 = 4.5x^3y^3 + 10.8x^2y^3 + 0.75xy^3 + 0.66xy^2$

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

Coumarin	M-polynomial
Isobergapten	$\mathcal{P}_1 = 3x^3y^3 + 8x^2y^3 + 2xy^3$ $\mathcal{P}_2 = 9x^3y^3 + 16x^2y^3 + 2xy^3$ $\mathcal{P}_3 = 9x^3y^3 + 24x^2y^3 + 6xy^3$ $\mathcal{P}_4 = 3 \cdot 3^{2p}x^3y^3 + 2 \cdot 3^{p}xy^3 + 8 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 8 \cdot 6^{-p}x^2y^3 + 2 \cdot 3^{-p}xy^3 + 3 \cdot 3^{-2p}x^3y^3$ $\mathcal{P}_6 = 6x^3y^3 + 17.33x^2y^3 + 6.66xy^3$ $\mathcal{P}_7 = 1.0x^3y^3 + 3.2x^2y^3 + 1xy^3$ $\mathcal{P}_8 = 4.5x^3y^3 + 9.6x^2y^3 + 1.5xy^3$
Isopimpinellin	$\mathcal{P}_1 = 2x^3y^3 + 10x^2y^3 + 1x^2y^2 + 1xy^3 + 2xy^2$ $\mathcal{P}_2 = 6x^3y^3 + 20x^2y^3 + 2x^2y^2 + 1xy^3 + 2xy^2$ $\mathcal{P}_3 = 6x^3y^3 + 30x^2y^3 + 2x^2y^2 + 3xy^3 + 4xy^2$ $\mathcal{P}_4 = 2^{2p}x^2y^2 + 2 \cdot 2^{p}xy^2 + 2 \cdot 3^{2p}x^3y^3 + 3^{p}xy^3 + 10 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 10 \cdot 6^{-p}x^2y^3 + 3^{-p}xy^3 + 2 \cdot 3^{-2p}x^3y^3 + 2 \cdot 2^{-p}xy^2 + 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 4x^3y^3 + 21.66x^2y^3 + 2x^2y^2 + 3.33xy^3 + 5xy^2$ $\mathcal{P}_7 = 0.66x^3y^3 + 4x^2y^3 + 0.5x^2y^2 + 0.5xy^3 + 1.33xy^2$ $\mathcal{P}_8 = 3x^3y^3 + 12x^2y^3 + 1x^2y^2 + 0.75xy^3 + 1.33xy^2$
Limettin	$\mathcal{P}_1 = 8x^4y^3 + 3x^3y^3 + 4x^2y^2 + 1xy^3$ $\mathcal{P}_2 = 32x^4y^3 + 9x^3y^3 + 8x^2y^2 + 1xy^3$ $\mathcal{P}_3 = 24x^4y^3 + 9x^3y^3 + 8x^2y^2 + 3xy^3$ $\mathcal{P}_4 = 8 \cdot 12^{p}x^4y^3 + 4 \cdot 2^{2p}x^2y^2 + 3 \cdot 3^{2p}x^3y^3 + 3^{p}xy^3$ $\mathcal{P}_5 = 3^{-p}xy^3 + 3 \cdot 3^{-2p}x^3y^3 + 4 \cdot 2^{-2p}x^2y^2 + 8 \cdot 12^{-p}x^4y^3$ $\mathcal{P}_6 = 16.66x^4y^3 + 6x^3y^3 + 8x^2y^2 + 3.33xy^3$ $\mathcal{P}_7 = 2.28x^4y^3 + 1x^3y^3 + 2x^2y^2 + 0.5xy^3$ $\mathcal{P}_8 = 13.71x^4y^3 + 4.5x^3y^3 + 4x^2y^2 + 0.75xy^3$

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

Coumarin	M-polynomial
Pimpinellin	$\mathcal{P}_1 = 2x^3y^3 + 9x^2y^3 + 3x^2y^2 + 1xy^3 + 1xy^2$ $\mathcal{P}_2 = 6x^3y^3 + 18x^2y^3 + 6x^2y^2 + 1xy^3 + 1xy^2$ $\mathcal{P}_3 = 6x^3y^3 + 27x^2y^3 + 6x^2y^2 + 3xy^3 + 2xy^2$ $\mathcal{P}_4 = 3 \cdot 2^{2p}x^2y^2 + 2^pxy^2 + 2 \cdot 3^{2p}x^3y^3 + 3^pxy^3 + 9 \cdot 6^px^2y^3$ $\mathcal{P}_5 = 9 \cdot 6^{-p}x^2y^3 + 3^{-p}xy^3 + 2 \cdot 3^{-2p}x^3y^3 + 2^{-p}xy^2 + 3 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 4x^3y^3 + 19.5x^2y^3 + 6x^2y^2 + 3.33xy^3 + 2.5xy^2$ $\mathcal{P}_7 = 0.66x^3y^3 + 3.6x^2y^3 + 1.5x^2y^2 + 0.5xy^3 + 0.66xy^2$ $\mathcal{P}_8 = 3x^3y^3 + 10.8x^2y^3 + 3x^2y^2 + 0.75xy^3 + 0.66xy^2$
Psoralen	$\mathcal{P}_1 = 4x^3y^3 + 10x^2y^3 + 5x^2y^2 + 3xy^3$ $\mathcal{P}_2 = 12x^3y^3 + 20x^2y^3 + 10x^2y^2 + 3xy^3$ $\mathcal{P}_3 = 12x^3y^3 + 30x^2y^3 + 10x^2y^2 + 9xy^3$ $\mathcal{P}_4 = 5 \cdot 2^{2p}x^2y^2 + 4 \cdot 3^{2p}x^3y^3 + 3 \cdot 3^pxy^3 + 10 \cdot 6^px^2y^3$ $\mathcal{P}_5 = 10 \cdot 6^{-p}x^2y^3 + 3 \cdot 3^{-p}xy^3 + 4 \cdot 3^{-2p}x^3y^3 + 5 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 8x^3y^3 + 21.66x^2y^3 + 10x^2y^2 + 10xy^3$ $\mathcal{P}_7 = 1.33x^3y^3 + 4x^2y^3 + 2.5x^2y^2 + 1.5xy^3$ $\mathcal{P}_8 = 6x^3y^3 + 12x^2y^3 + 5x^2y^2 + 2.25xy^3$
Skimmin	$\mathcal{P}_1 = 4x^3y^3 + 9x^2y^3 + 3x^2y^2 + 1xy^3 + 1xy^2$ $\mathcal{P}_2 = 12x^3y^3 + 18x^2y^3 + 6x^2y^2 + 1xy^3 + 1xy^2$ $\mathcal{P}_3 = 12x^3y^3 + 27x^2y^3 + 6x^2y^2 + 3xy^3 + 2xy^2$ $\mathcal{P}_4 = 3 \cdot 2^{2p}x^2y^2 + 2^pxy^2 + 4 \cdot 3^{2p}x^3y^3 + 3^pxy^3 + 9 \cdot 6^px^2y^3$ $\mathcal{P}_5 = 9 \cdot 6^{-p}x^2y^3 + 3^{-p}xy^3 + 4 \cdot 3^{-2p}x^3y^3 + 2^{-p}xy^2 + 3 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 8x^3y^3 + 19.5x^2y^3 + 6x^2y^2 + 3.33xy^3 + 2.5xy^2$ $\mathcal{P}_7 = 1.33x^3y^3 + 3.6x^2y^3 + 1.5x^2y^2 + 0.5xy^3 + 0.66xy^2$ $\mathcal{P}_8 = 6x^3y^3 + 10.8x^2y^3 + 3x^2y^2 + 0.75xy^3 + 0.66xy^2$

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Table 7: M-polynomials of molecular graphs of coumarins.

Coumarin	M-polynomial
Umbelliferon	$\mathcal{P}_1 = 6x^3y^3 + 8x^2y^3 + 3x^2y^2 + 1xy^3 + 2xy^2$ $\mathcal{P}_2 = 18x^3y^3 + 16x^2y^3 + 6x^2y^2 + 1xy^3 + 2xy^2$ $\mathcal{P}_3 = 18x^3y^3 + 24x^2y^3 + 6x^2y^2 + 3xy^3 + 4xy^2$ $\mathcal{P}_4 = 3 \cdot 2^{2p}x^2y^2 + 2 \cdot 2^{p}xy^2 + 6 \cdot 3^{2p}x^3y^3 + 3^{p}xy^3 + 8 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 8 \cdot 6^{-p}x^2y^3 + 3^{-p}xy^3 + 6 \cdot 3^{-2p}x^3y^3 + 2 \cdot 2^{-p}xy^2 + 3 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 12x^3y^3 + 17.33x^2y^3 + 6x^2y^2 + 3.33xy^3 + 5xy^2$ $\mathcal{P}_7 = 2x^3y^3 + 3.2x^2y^3 + 1.5x^2y^2 + 0.5xy^3 + 1.33xy^2$ $\mathcal{P}_8 = 9x^3y^3 + 9.6x^2y^3 + 3x^2y^2 + 0.75xy^3 + 1.33xy^2$
Angelicin	$\mathcal{P}_1 = 6x^3y^3 + 8x^2y^3 + 3x^2y^2 + 1xy^3 + 2xy^2$ $\mathcal{P}_2 = 18x^3y^3 + 16x^2y^3 + 6x^2y^2 + 1xy^3 + 2xy^2$ $\mathcal{P}_3 = 18x^3y^3 + 24x^2y^3 + 6x^2y^2 + 3xy^3 + 4xy^2$ $\mathcal{P}_4 = 3 \cdot 2^{2p}x^2y^2 + 2 \cdot 2^{p}xy^2 + 6 \cdot 3^{2p}x^3y^3 + 3^{p}xy^3 + 8 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 8 \cdot 6^{-p}x^2y^3 + 3^{-p}xy^3 + 6 \cdot 3^{-2p}x^3y^3 + 2 \cdot 2^{-p}xy^2 + 3 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 12x^3y^3 + 17.33x^2y^3 + 6x^2y^2 + 3.33xy^3 + 5xy^2$ $\mathcal{P}_7 = 2x^3y^3 + 3.2x^2y^3 + 1.5x^2y^2 + 0.5xy^3 + 1.33xy^2$ $\mathcal{P}_8 = 9x^3y^3 + 9.6x^2y^3 + 3x^2y^2 + 0.75xy^3 + 1.33xy^2$
Bergapten	$\mathcal{P}_1 = 2x^3y^3 + 10x^2y^3 + 3x^2y^2 + 1xy^3$ $\mathcal{P}_2 = 6x^3y^3 + 20x^2y^3 + 6x^2y^2 + 1xy^3$ $\mathcal{P}_3 = 6x^3y^3 + 30x^2y^3 + 6x^2y^2 + 3xy^3$ $\mathcal{P}_4 = 3 \cdot 2^{2p}x^2y^2 + 2 \cdot 3^{2p}x^3y^3 + 3^{p}xy^3 + 10 \cdot 6^{p}x^2y^3$ $\mathcal{P}_5 = 10 \cdot 6^{-p}x^2y^3 + 3^{-p}xy^3 + 2 \cdot 3^{-2p}x^3y^3 + 3 \cdot 2^{-2p}x^2y^2$ $\mathcal{P}_6 = 4x^3y^3 + 21.66x^2y^3 + 6x^2y^2 + 3.33xy^3$ $\mathcal{P}_7 = 0.66x^3y^3 + 4x^2y^3 + 1.5x^2y^2 + 0.5xy^3$ $\mathcal{P}_8 = 3x^3y^3 + 12x^2y^3 + 3x^2y^2 + 0.75xy^3$

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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).

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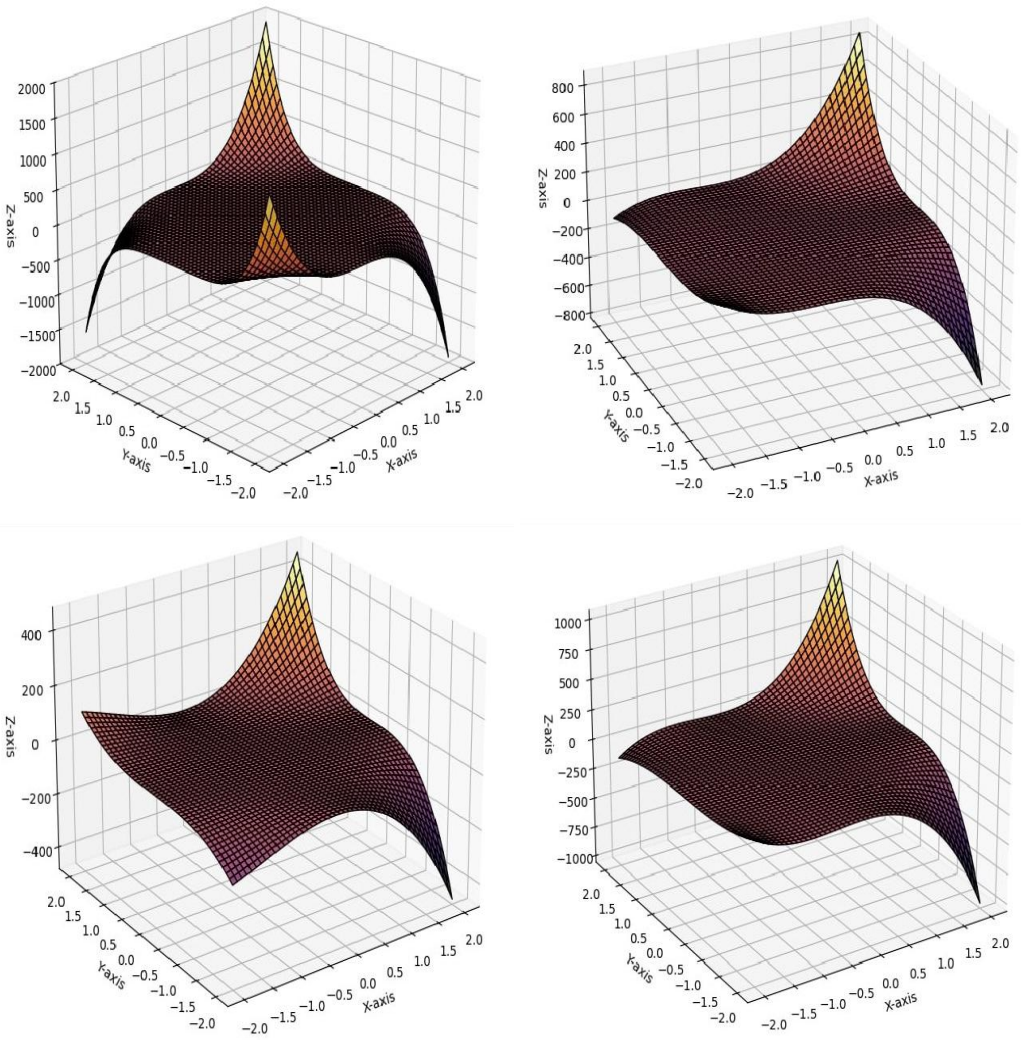

Figure 2: 3D plots of M-polynomials of molecular graphs of coumarins

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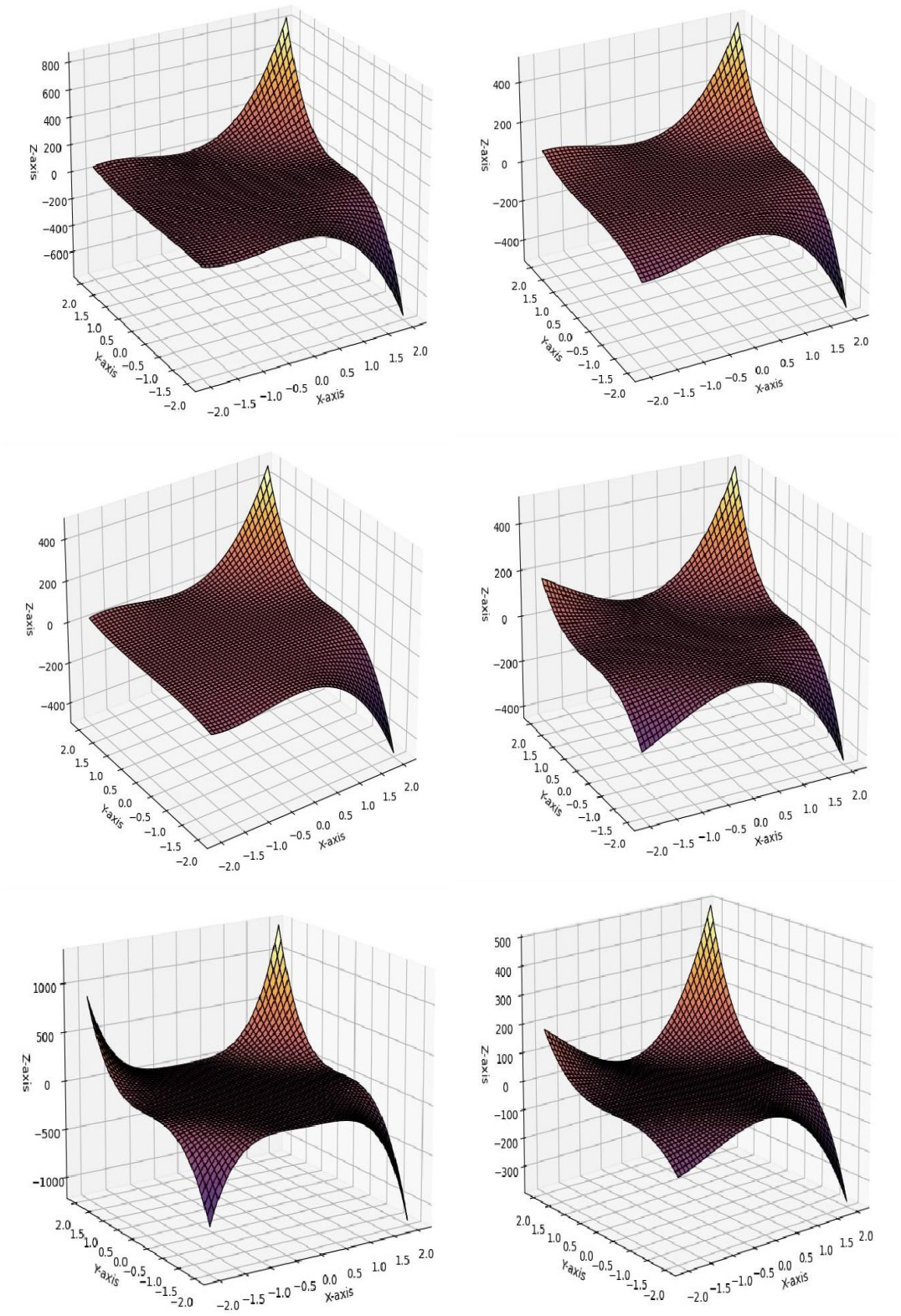

Figure 3: 3D plots of M-polynomials of molecular graphs of coumarins.

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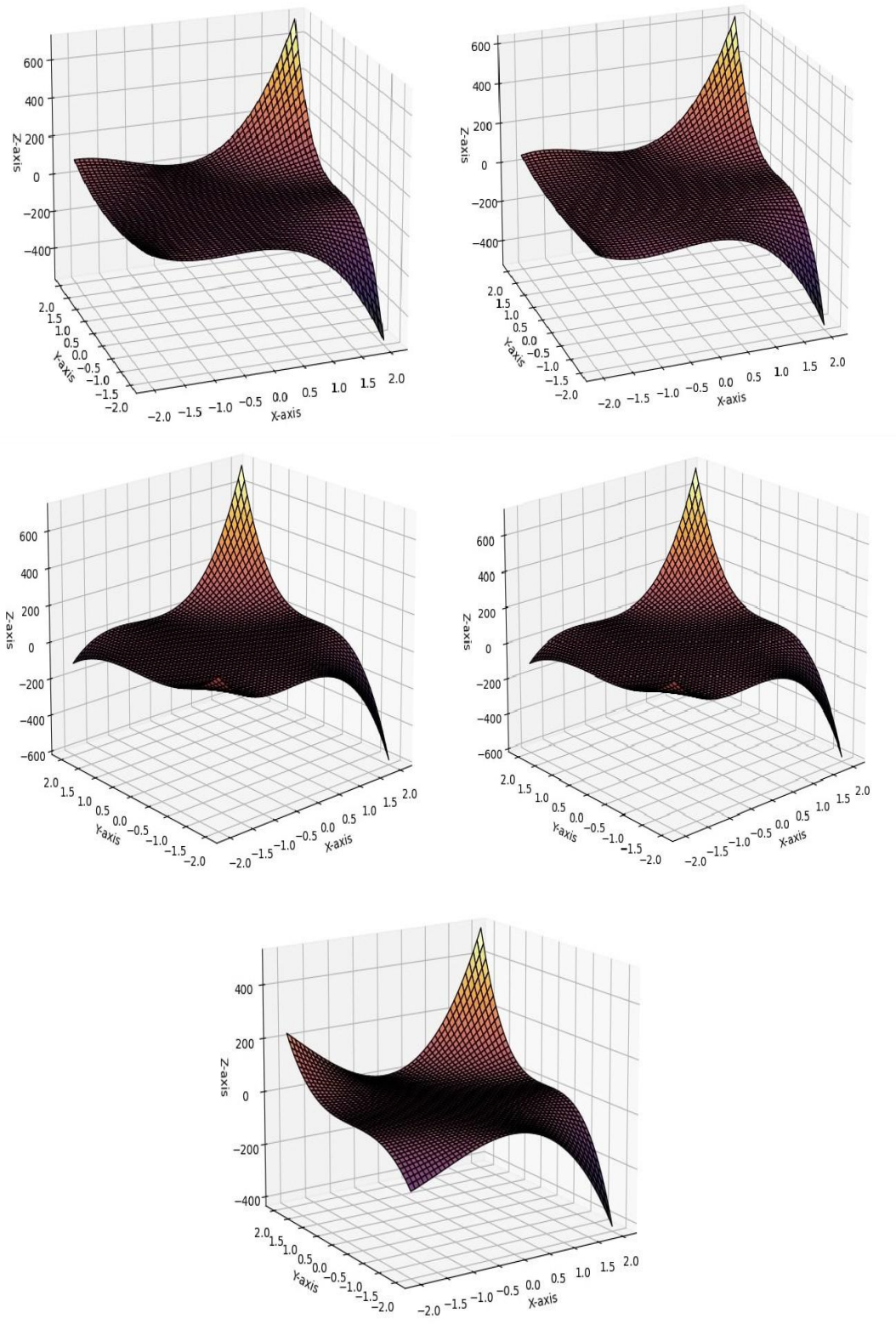

Figure 4: 3D plots of M-polynomials of molecular graphs of coumarins.

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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 8: 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

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

Table 9: Topological indices for molecular graphs of coumarins

Drugs	$R_p(G)$	$RR_p(G)$	$SSD(G)$	$H(G)$	$I(G)$
Daphnetin	$3^{2p+1}+6^{p+1}+2^{2p+1}+3^{p+1}$	$3^{1-2p}+6^{1-p}+2^{1-2p}+3^{1-p}$	33.00	5.90	15.95
Daphnin	$2\cdot 2^{2p}+6\cdot 3^{2p}+6\cdot 3^{p}+11\cdot 6^{p}$	$11\cdot 6^{-p}+6\cdot 3^{-p}+6\cdot 3^{-2p}+2\cdot 2^{-2p}$	59.83	10.4	28.7
Esculetin	$2\cdot 3^{2p}+3\cdot 3^{p}+9\cdot 6^{p}$	$9\cdot 6^{-p}+3\cdot 3^{-p}+2\cdot 3^{-2p}$	33.5	5.76	16.05
Esculin	$2^{p}+8\cdot 3^{2p}+4\cdot 3^{p}+14\cdot 6^{p}$	$14\cdot 6^{-p}+4\cdot 3^{-p}+8\cdot 3^{-2p}+2^{-p}$	62.16	10.93	32.46
Herniarin	$2^{p}+3\cdot 3^{2p}+3^{p}+9\cdot 6^{p}$	$9\cdot 6^{-p}+3^{-p}+3\cdot 3^{-2p}+2^{-p}$	31.33	5.76	16.71
Imperatorin	$5\cdot 2^{2p}+4\cdot 3^{2p}+3\cdot 3^{p}+10\cdot 6^{p}$	$10\cdot 6^{-p}+3\cdot 3^{-p}+4\cdot 3^{-2p}+5\cdot 2^{-2p}$	49.66	9.33	25.25
Isobergapten	$3\cdot 2^{2p}+2^{p}+4\cdot 3^{2p}+3^{p}+9\cdot 6^{p}$	$9\cdot 6^{-p}+3^{-p}+4\cdot 3^{-2p}+2^{-p}+3\cdot 2^{-2p}$	39.33	7.6	21.21
Isopimpinellin	$3\cdot 2^{2p}+2\cdot 2^{p}+6\cdot 3^{2p}+3^{p}+8\cdot 6^{p}$	$8\cdot 6^{-p}+3^{-p}+6\cdot 3^{-2p}+2\cdot 2^{-p}+3\cdot 2^{-2p}$	43.66	8.53	23.68
Limettin	$2^{2p}+2\cdot 2^{p}+2\cdot 3^{2p}+3^{p}+10\cdot 6^{p}$	$10\cdot 6^{-p}+3^{-p}+2\cdot 3^{-2p}+2\cdot 2^{-p}+2^{-2p}$	36	7	18.08
Pimpinellin	$3\cdot 2^{2p}+2\cdot 2^{p}+6\cdot 3^{2p}+3^{p}+8\cdot 6^{p}$	$8\cdot 6^{-p}+3^{-p}+6\cdot 3^{-2p}+2\cdot 2^{-p}+3\cdot 2^{-2p}$	43.66	8.53	23.68
Psoralen	$3\cdot 2^{2p}+2\cdot 3^{2p}+3^{p}+10\cdot 6^{p}$	$10\cdot 6^{-p}+3^{-p}+2\cdot 3^{-2p}+3\cdot 2^{-2p}$	35.00	6.6	18.75
Skimmin	$2\cdot 2^{2p}+2^{p}+5\cdot 3^{2p}+4\cdot 3^{p}+13\cdot 6^{p}$	$13\cdot 6^{-p}+4\cdot 3^{-p}+5\cdot 3^{-2p}+2^{-p}+2\cdot 2^{-2p}$	58.00	10.53	28.76
Umbelliferon	$3\cdot 3^{2p}+2\cdot 3^{p}+8\cdot 6^{p}$	$8\cdot 6^{-p}+2\cdot 3^{-p}+3\cdot 3^{-2p}$	30.00	5.2	15.6
Angelicin	$8\cdot 12^{p}+4\cdot 2^{2p}+3\cdot 3^{2p}+3^{p}$	$3^{-p}+3\cdot 3^{-2p}+4\cdot 2^{-2p}+8\cdot 12^{-p}$	34.00	5.78	22.96
Bergapten	$3\cdot 2^{2p}+2^{p}+2\cdot 3^{2p}+3^{p}+9\cdot 6^{p}$	$9\cdot 6^{-p}+3^{-p}+2\cdot 3^{-2p}+2^{-p}+3\cdot 2^{-2p}$	35.33	6.93	18.21

5.1 Regression Modules

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

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properties of coumarins (see Table 8). The QSPR models for the various physicochemical properties of coumarin drugs with the best-fitting topological indices are given by:

Linear Regression for SDD(G) :

$$BP = 9.631(SDD(G)) + 58.591$$
$$n = 15 \quad \mathbf{r = 0.918} \quad F = 69.698 \quad SF = 46.922 \quad Sig = 0.000$$
$$VP = 0.042(SDD(G)) + (-0.546)$$
$$n = 15 \quad \mathbf{r = 0.906} \quad F = 59.857 \quad SF = 0.221 \quad Sig = 0.000$$
$$FP = 2.806(SDD(G)) + 87.183$$
$$n = 15 \quad \mathbf{r = 0.900} \quad F = 55.648 \quad SF = 15.296 \quad Sig = 0.000$$
$$MR = 1.151(SDD(G)) + 10.277$$
$$n = 15 \quad \mathbf{r = 0.958} \quad F = 146.391 \quad SF = 3.870 \quad Sig = 0.000$$
$$P = 0.456(SDD(G)) + 4.117$$
$$n = 15 \quad \mathbf{r = 0.959} \quad F = 149.823 \quad SF = 1.514 \quad Sig = 0.000$$

Linear Regression for H(G):

$$MR = 6.606(H(G)) + 7.626$$
$$n = 15 \quad \mathbf{r = 0.981} \quad F = 328.733 \quad SF = 2.643 \quad Sig = 0.000$$
$$P = 2.613(H(G)) + 3.078$$
$$n = 15 \quad \mathbf{r = 0.981} \quad F = 336.732 \quad SF = 1.033 \quad Sig = 0.000$$
$$MV = 17.183(H(G)) + 30.083$$
$$n = 15 \quad \mathbf{r = 0.935} \quad F = 90.298 \quad SF = 13.117 \quad Sig = 0.000$$

Linear Regression for I(G):

$$MR = 2.349(I(G)) + 6.663$$
$$n = 15 \quad \mathbf{r = 0.944} \quad F = 97.340 \quad SF = 4.669 \quad Sig = 0.000$$
$$P = 0.929(I(G)) + 2.707$$
$$n = 15 \quad \mathbf{r = 0.944} \quad F = 97.670 \quad SF = 4.843 \quad Sig = 0.000$$

Quadratic Regression for SDD(G):

$$BP = (0.356)(SDD(G))^2 + (-23.176)(SDD(G)) + (767.554)$$
$$n = 15 \quad \mathbf{r = 0.955} \quad F = 62.510 \quad SF = 36.453 \quad Sig = 0.000$$
$$VP = (0.002)(SDD(G))^2 + (-0.133)(SDD(G)) + (3.237)$$
$$n = 15 \quad \mathbf{r = 0.961} \quad F = 71.630 \quad SF = 0.152 \quad Sig = 0.000$$
$$E = (0.062)(SDD(G))^2 + (-4.381)(SDD(G)) + (142.527)$$
$$n = 15 \quad \mathbf{r = 0.954} \quad F = 60.629 \quad SF = 5.130 \quad Sig = 0.000$$
$$FP = (-0.048)(SDD(G))^2 + (7.236)(SDD(G)) + (-8.561)$$
$$n = 15 \quad \mathbf{r = 0.908} \quad F = 28.290 \quad SF = 15.304 \quad Sig = 0.000$$
$$MR = (-0.032)(SDD(G))^2 + (4.116)(SDD(G)) + (-53.795)$$
$$n = 15 \quad \mathbf{r = 0.981} \quad F = 151.137 \quad SF = 2.756 \quad Sig = 0.000$$
$$PSA = (0.172)(SDD(G))^2 + (-12.787)(SDD(G)) + (282.971)$$
$$n = 15 \quad \mathbf{r = 0.951} \quad F = 56.497 \quad SF = 12.804 \quad Sig = 0.000$$
$$P = (-0.013)(SDD(G))^2 + (1.619)(SDD(G)) + (-21.028)$$

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$$n = 15 \quad \mathbf{r = 0.981} \quad F = 155.759 \quad SF = 1.074 \quad Sig = 0.000$$

$$MV = (-0.140)(SDD(G))^2 + (15.795)(SDD(G)) + (-237.387)$$

$$n = 15 \quad \mathbf{r = 0.940} \quad F = 45.469 \quad SF = 13.140 \quad Sig = 0.000$$

Quadratic Regression for H(G):

$$BP = (16.478)(H(G))^2 + (-215.947)(H(G)) + (1089.222)$$

$$n = 15 \quad \mathbf{r = 0.944} \quad F = 49.099 \quad SF = 40.648 \quad Sig = 0.000$$

$$VP = (0.079)(H(G))^2 + (-1.054)(H(G)) + (4.387)$$

$$n = 15 \quad \mathbf{r = 0.942} \quad F = 47.230 \quad SF = 0.183 \quad Sig = 0.000$$

$$E = (2.623)(H(G))^2 + (-35.666)(H(G)) + (184.079)$$

$$n = 15 \quad \mathbf{r = 0.942} \quad F = 47.636 \quad SF = 5.717 \quad Sig = 0.000$$

$$MR = (-0.174)(H(G))^2 + (9.406)(H(G)) + (-3.031)$$

$$n = 15 \quad \mathbf{r = 0.982} \quad F = 157.921 \quad SF = 2.698 \quad Sig = 0.000$$

$$PSA = (6.648)(H(G))^2 + (-91.770)(H(G)) + (357.671)$$

$$n = 15 \quad \mathbf{r = 0.929} \quad F = 37.923 \quad SF = 15.274 \quad Sig = 0.000$$

$$P = (-0.066)(H(G))^2 + (3.674)(H(G)) + (-0.961)$$

$$n = 15 \quad \mathbf{r = 0.982} \quad F = 161.367 \quad SF = 1.056 \quad Sig = 0.000$$

$$MV = (-2.233)(H(G))^2 + (53.214)(H(G)) + (-107.060)$$

$$n = 15 \quad \mathbf{r = 0.952} \quad F = 57.925 \quad SF = 11.790 \quad Sig = 0.000$$

Quadratic Regression for I(G):

$$BP = (1.871)(I(G))^2 + (-68.877)(I(G)) + (1021.469)$$

$$n = 15 \quad \mathbf{r = 0.919} \quad F = 49.099 \quad SF = 40.648 \quad Sig = 0.000$$

$$VP = (0.009)(I(G))^2 + (-0.336)(I(G)) + (4.047)$$

$$n = 15 \quad \mathbf{r = 0.926} \quad F = 32.953 \quad SF = 0.214 \quad Sig = 0.000$$

$$E = (0.291)(I(G))^2 + (-11.093)(I(G)) + (169.782)$$

$$n = 15 \quad \mathbf{r = 0.918} \quad F = 29.649 \quad SF = 7.003 \quad Sig = 0.000$$

$$MR = (-0.040)(I(G))^2 + (4.191)(I(G)) + (-13.485)$$

$$n = 15 \quad \mathbf{r = 0.947} \quad F = 47.535 \quad SF = 4.741 \quad Sig = 0.000$$

$$PSA = (0.723)(I(G))^2 + (-27.941)(I(G)) + (314.157)$$

$$n = 15 \quad \mathbf{r = 0.905} \quad F = 24.941 \quad SF = 18.171 \quad Sig = 0.000$$

$$P = (-0.015)(I(G))^2 + (1.638)(I(G)) + (-5.048)$$

$$n = 15 \quad \mathbf{r = 0.947} \quad F = 47.543 \quad SF = 1.874 \quad Sig = 0.000$$

Cubic Regression for SDD(G) :

$$BP = (0.004)(SDD(G))^3 + (5.437)(SDD(G))^2 + (-0.179)SDD(G)) + (442.768)$$

$$n = 15 \quad \mathbf{r = 0.963} \quad F = 76.849 \quad SF = 0.147 \quad Sig = 0.000$$

$$VP = (2.284 \times 10^{-5})(SDD(G))^3 + (7.131)(SDD(G))^2 + (-0.001)SDD(G)) + (1.374)$$

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

$$E = (0.001)(SDD(G))^3 + (3.323)(SDD(G))^2 + (-0.038)SDD(G)) + (80.518)$$

$$n = 15 \quad \mathbf{r = 0.955} \quad F = 62.815 \quad SF = 5.048 \quad Sig = 0.000$$

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$$FP = (-0.048)(SDD(G))^3 + (7.000)(SDD(G))^2 + (7.236)SDD(G)) + (-8.561)$$

$$n = 15 \quad \mathbf{r = 0.908} \quad F = 28.290 \quad SF = 15.304 \quad Sig = 0.000$$

$$MR = (0.000)(SDD(G))^3 + (6.804)(SDD(G))^2 + (2.709)SDD(G)) + (-33.916)$$

$$n = 15 \quad \mathbf{r = 0.981} \quad F = 154.896 \quad SF = 2.723 \quad Sig = 0.000$$

$$PSA = (0.002)(SDD(G))^3 + (4.748)(SDD(G))^2 + (-0.120)SDD(G)) + (102.270)$$

$$n = 15 \quad \mathbf{r = 0.953} \quad F = 59.715 \quad SF = 12.487 \quad Sig = 0.000$$

$$P = (-9.336 \times 10^{-5})(SDD(G))^3 + (6.497)(SDD(G))^2 + (1.067)SDD(G)) + (-13.221)$$

$$n = 15 \quad \mathbf{r = 0.982} \quad F = 159.556 \quad SF = 1.061 \quad Sig = 0.000$$

$$MV = (-0.001)(SDD(G))^3 + (17.005)(SDD(G))^2 + (9.701)SDD(G)) + (-151.736)$$

$$n = 15 \quad \mathbf{r = 0.942} \quad F = 47.000 \quad SF = 12.949 \quad Sig = 0.000$$

Cubic Regression for H(G):

$$BP = (1.172)(H(G))^3 + (5.949)(H(G))^2 + (-11.517)H(G)) + (551.213)$$

$$n = 15 \quad \mathbf{r = 0.948} \quad F = 52.801 \quad SF = 39.347 \quad Sig = 0.000$$

$$VP = (0.006)(H(G))^3 + (7.993)(H(G))^2 + (-0.058)H(G)) + (1.767)$$

$$n = 15 \quad \mathbf{r = 0.947} \quad F = 52.270 \quad SF = 0.175 \quad Sig = 0.000$$

$$E = (0.193)(H(G))^3 + (5.837)(H(G))^2 + (-1.991)H(G)) + (95.031)$$

$$n = 15 \quad \mathbf{r = 0.947} \quad F = 51.987 \quad SF = 5.499 \quad Sig = 0.000$$

$$MR = (-0.008)(H(G))^3 + (12.056)(H(G))^2 + (8.190)H(G)) + (-0.312)$$

$$n = 15 \quad \mathbf{r = 0.982} \quad F = 159.258 \quad SF = 2.687 \quad Sig = 0.000$$

$$PSA = (0.500)(H(G))^3 + (8.975)(H(G))^2 + (-5.275)H(G)) + (129.569)$$

$$n = 15 \quad \mathbf{r = 0.936} \quad F = 42.399 \quad SF = 14.550 \quad Sig = 0.000$$

$$P = (-0.003)(H(G))^3 + (11.867)(H(G))^2 + (3.215)H(G)) + (-13.221)$$

$$n = 15 \quad \mathbf{r = 0.982} \quad F = 159.556 \quad SF = 1.061 \quad Sig = 0.000$$

$$MV = (-0.001)(H(G))^3 + (17.005)(H(G))^2 + (9.701)H(G)) + (0.062)$$

$$n = 15 \quad \mathbf{r = 0.982} \quad F = 162.682 \quad SF = 1.051 \quad Sig = 0.000$$

Cubic Regression for H(G):

$$BP = (0.025)(I(G))^3 + (41.667)(I(G))^2 + (-24.283)I(G)) + (680.323)$$

$$n = 15 \quad \mathbf{r = 0.913} \quad F = 27.394 \quad SF = 52.262 \quad Sig = 0.000$$

$$VP = (0.000)(I(G))^3 + (38.359)(I(G))^2 + (-0.124)I(G)) + (2.432)$$

$$n = 15 \quad \mathbf{r = 0.920} \quad F = 30.184 \quad SF = 0.222 \quad Sig = 0.000$$

$$E = (0.004)(I(G))^3 + (44.718)(I(G))^2 + (-4.171)I(G)) + (44.718)$$

$$n = 15 \quad \mathbf{r = 0.911} \quad F = 26.853 \quad SF = 7.299 \quad Sig = 0.000$$

$$MR = (-0.001)(I(G))^3 + (18.206)(I(G))^2 + (3.347)I(G)) + (-7.745)$$

$$n = 15 \quad \mathbf{r = 0.947} \quad F = 48.066 \quad SF = 4.717 \quad Sig = 0.000$$

$$P = (0.000)(I(G))^3 + (18.179)(I(G))^2 + (1.313)I(G)) + (-2.848)$$

$$n = 15 \quad \mathbf{r = 0.947} \quad F = 48.061 \quad SF = 1.865 \quad Sig = 0.000$$

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

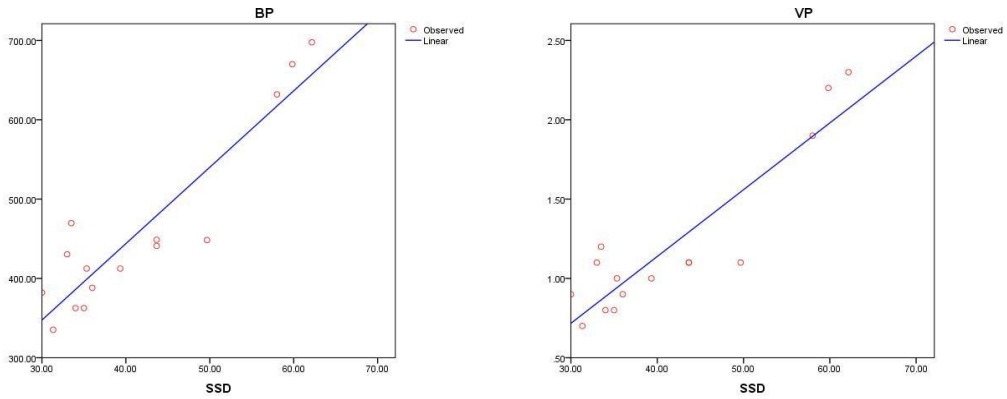

Figure 5: Linear regression model of BP and VP with *SDD*(*G*)

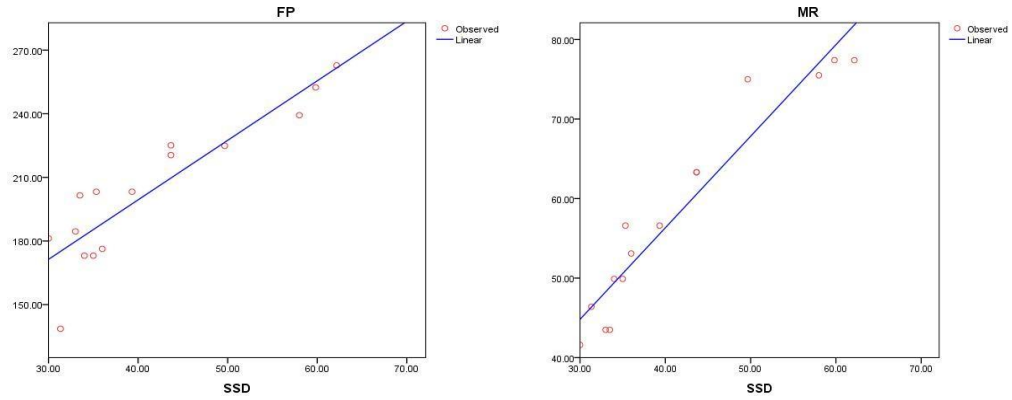

Figure 6: Linear regression model of FP and MR with *SDD*(*G*)

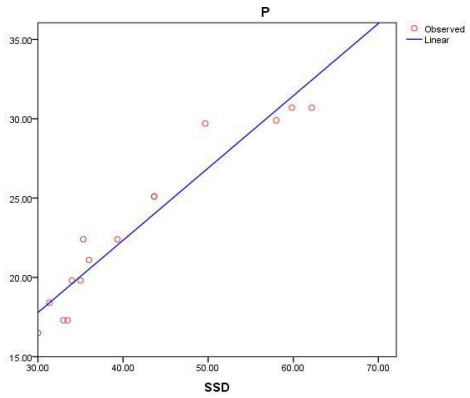

Figure 7: Linear regression model of P with *SDD*(*G*)

DOI: https://doi.org/10.71058/jodac.v9i6013

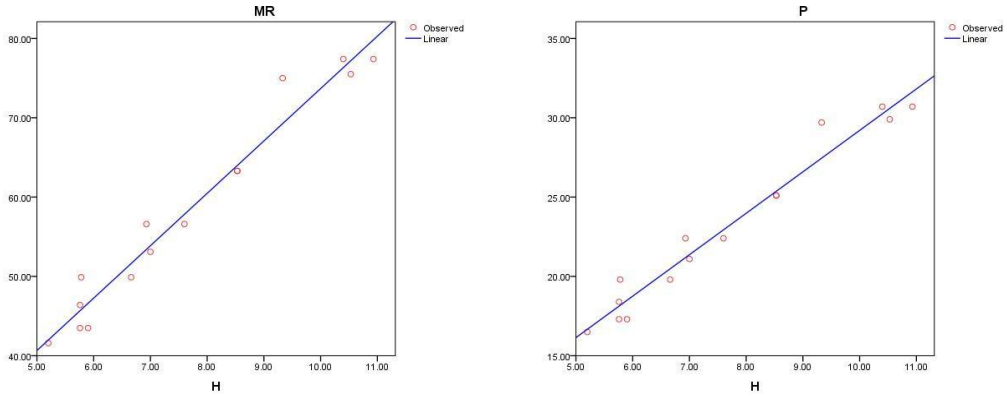

Figure 8: Linear regression model of MR and P with $H(G)$

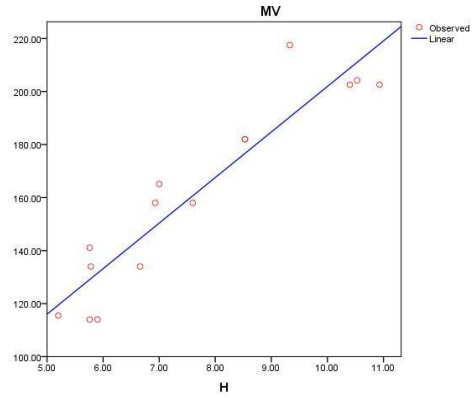

Figure 9: Linear regression model of MV with H(G)

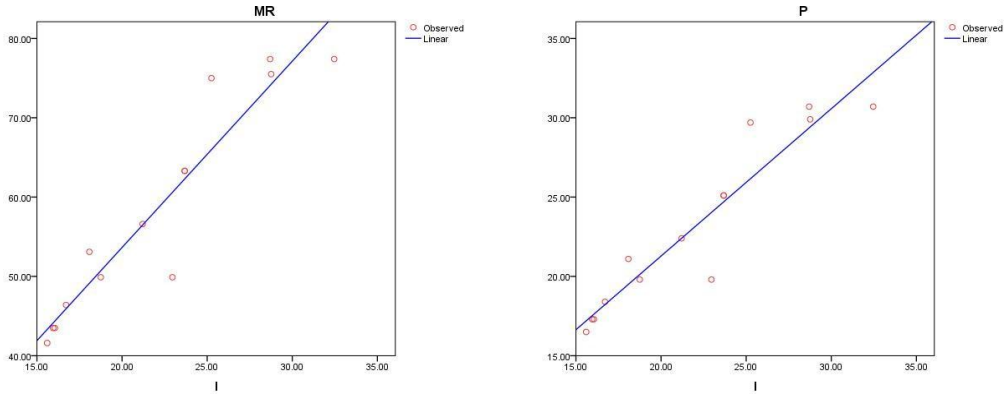

Figure 10: Linear regression model of MR and P with $I(G)$

DOI: https://doi.org/10.71058/jodac.v9i6013

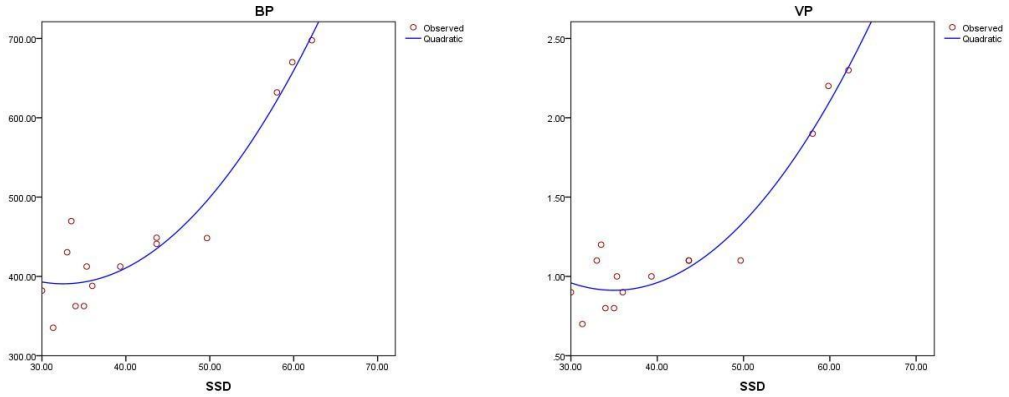

Figure 11: Quadratic regression model of BP and VP with SDD(G)

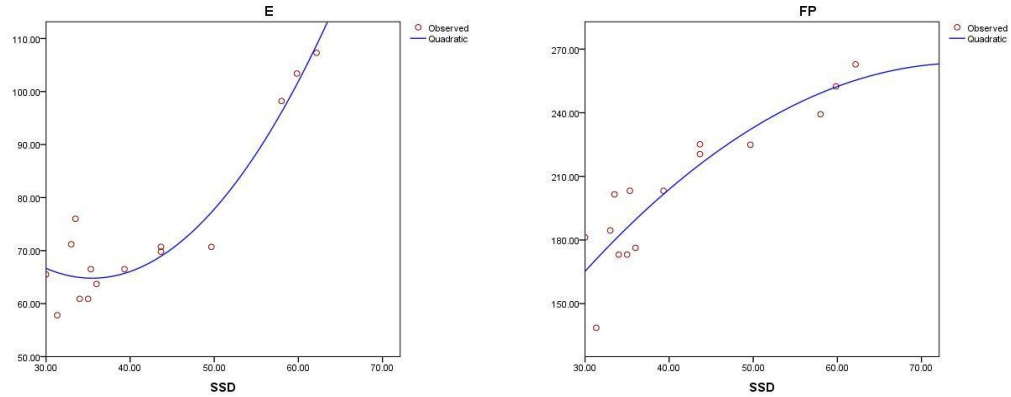

Figure 12: Quadratic regression model of E and FP with *SDD*(*G*)

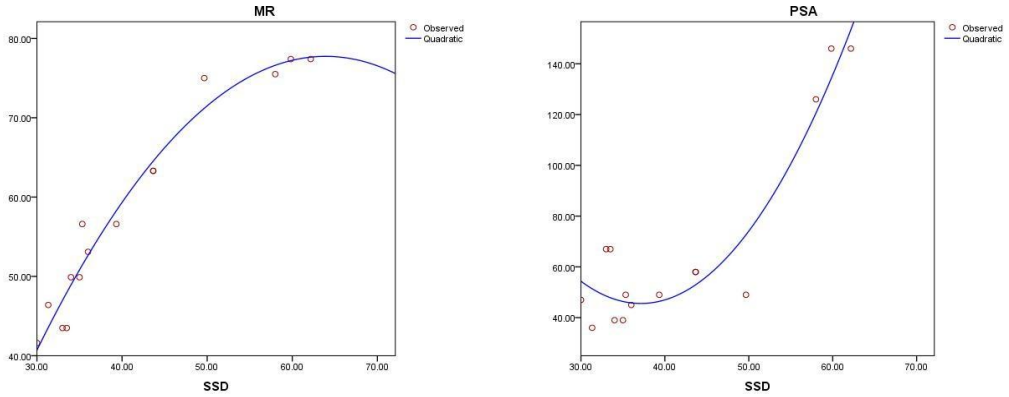

Figure 13: Quadratic regression model of MR and PSA with *SDD*(*G*)

DOI: https://doi.org/10.71058/jodac.v9i6013

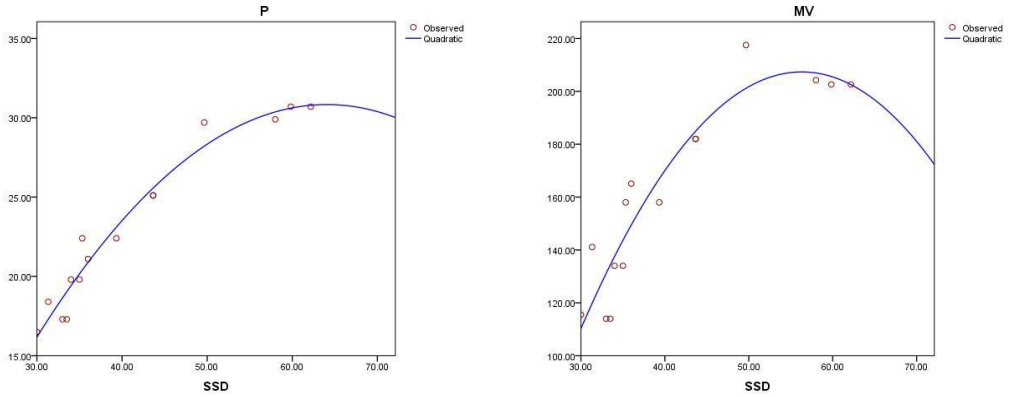

Figure 14: Quadratic regression model of P and MV with SDD(G)

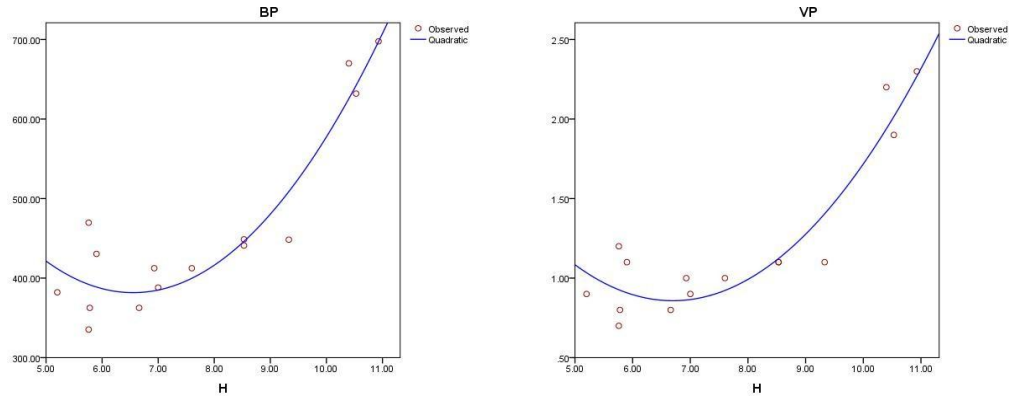

Figure 15: Quadratic regression model of BP and VP with H(G)

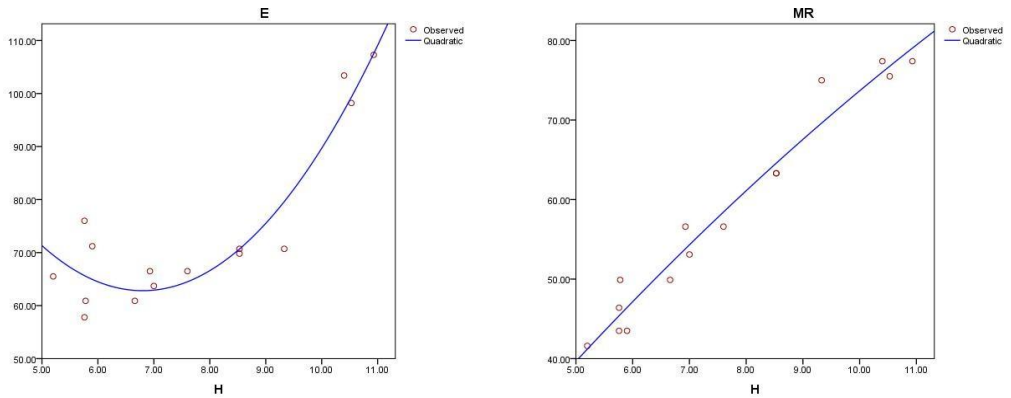

Figure 16: Quadratic regression model of E and MR with *H*(*G*)

DOI: https://doi.org/10.71058/jodac.v9i6013

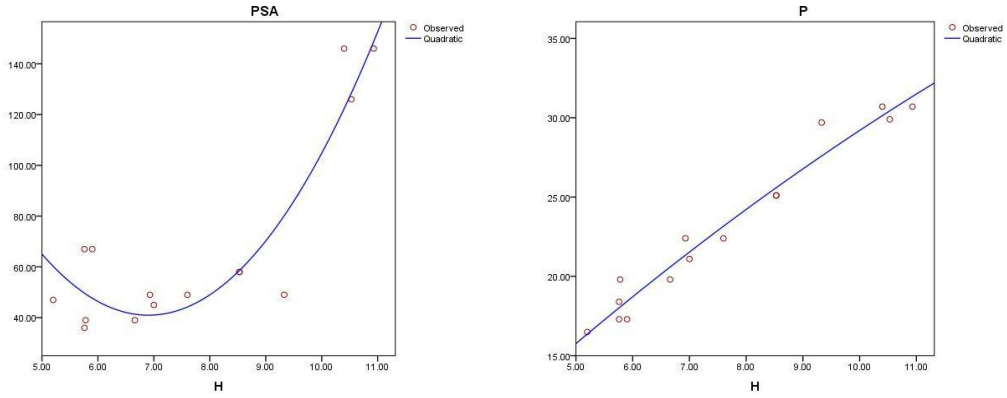

Figure 17: Quadratic regression model of PSA and P with H(G)

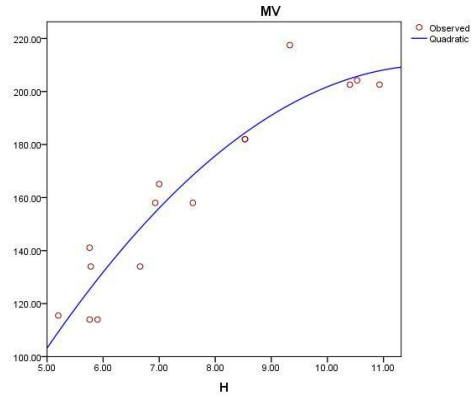

Figure 18: Quadratic regression model of MV with H(G)

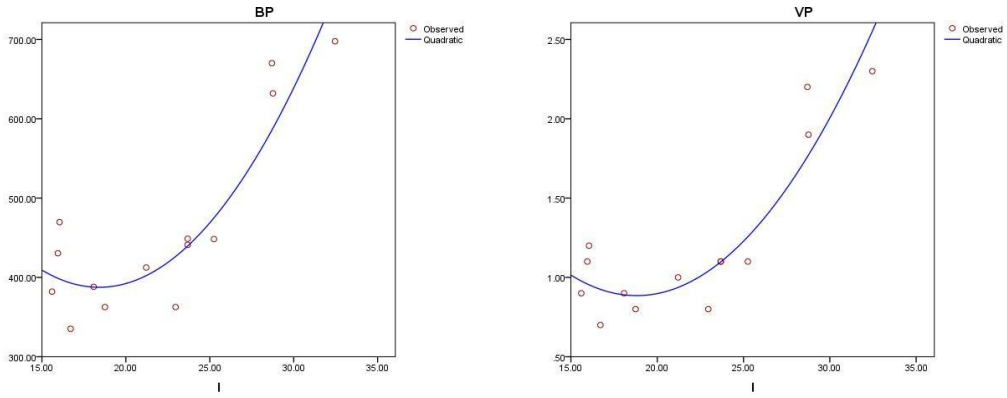

Figure 19: Quadratic regression model of BP and VP with *I*(*G*)

DOI: https://doi.org/10.71058/jodac.v9i6013

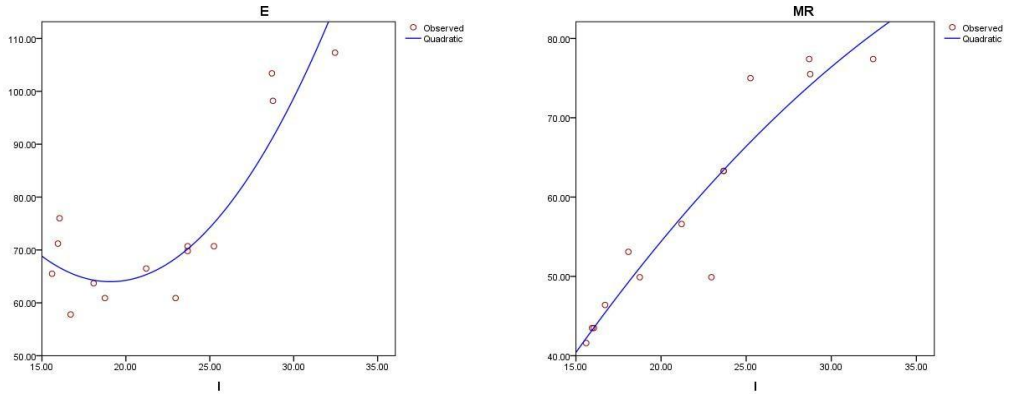

Figure 20: Quadratic regression model of E and MR with I(G)

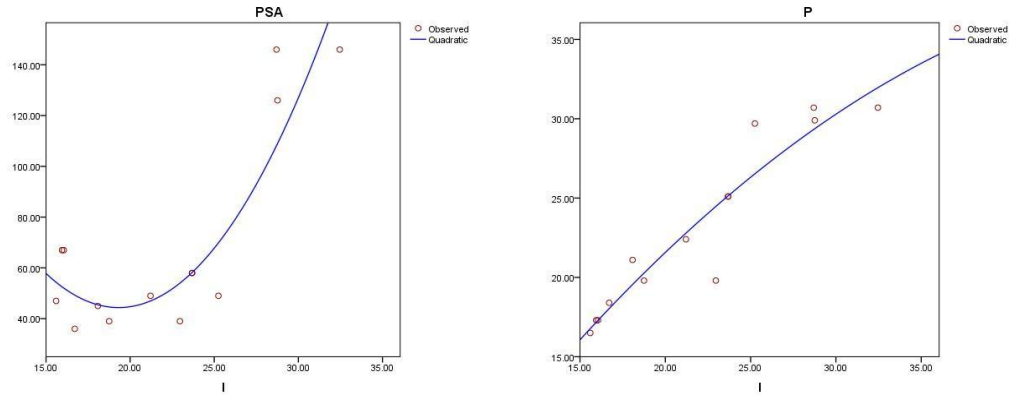

Figure 21: Quadratic regression model of PSA and P with *I*(*G*)

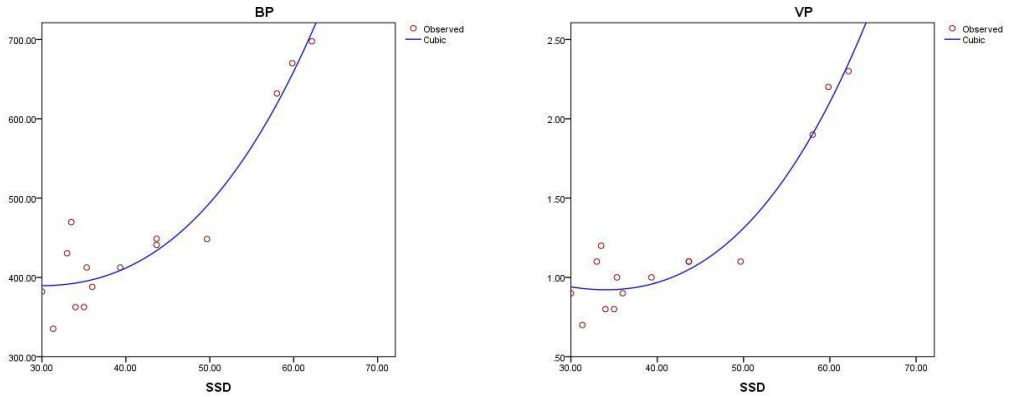

Figure 22: Cubic regression model of BP and VP with *SDD*(*G*)

DOI: https://doi.org/10.71058/jodac.v9i6013

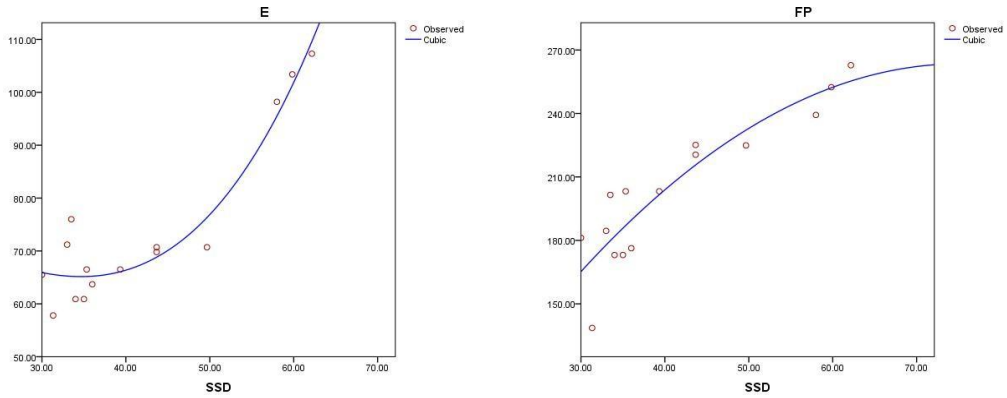

Figure 23: Cubic regression model of E and FP with *SDD*(*G*)

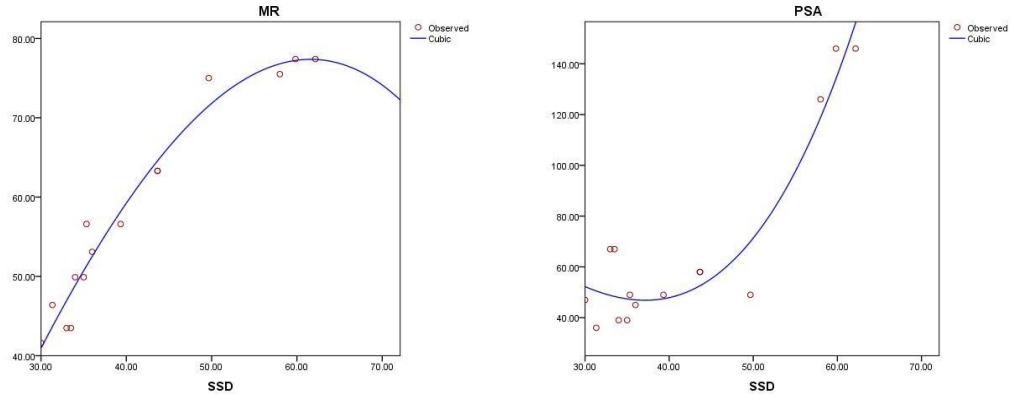

Figure 24: Cubic regression model of MR and PSA with SDD(G)

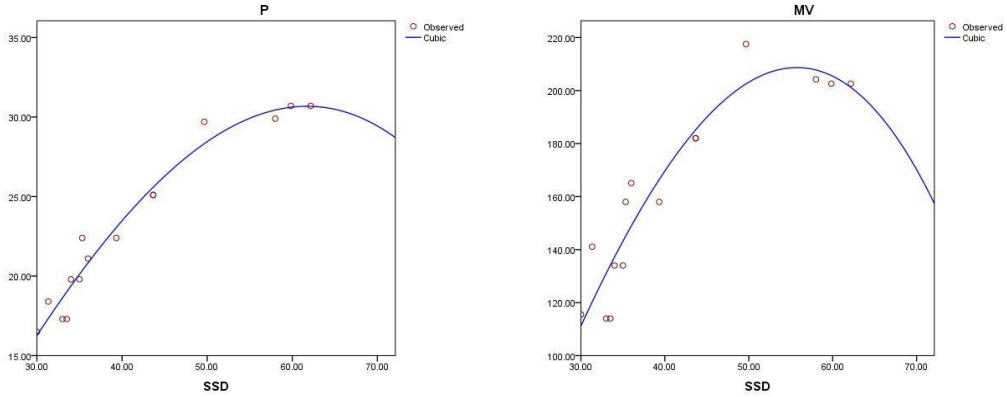

Figure 25: Cubic regression model of P and MV with SDD(G)

DOI: https://doi.org/10.71058/jodac.v9i6013

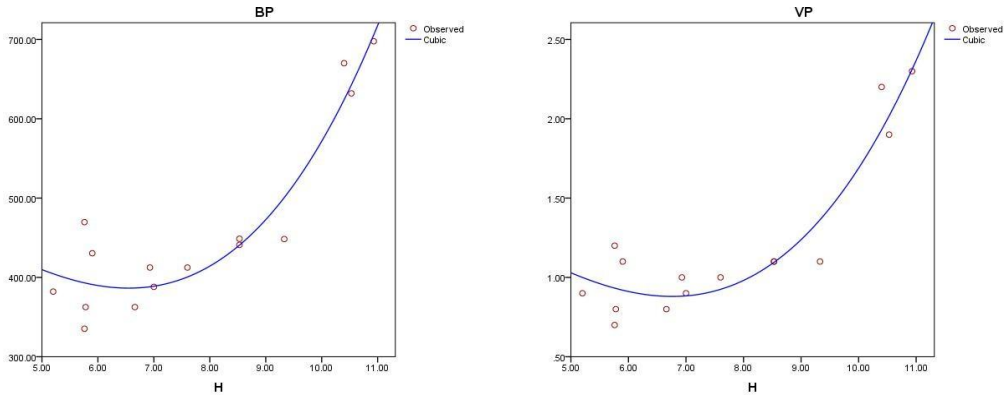

Figure 26: Cubic regression model of BP and VP with H(G)

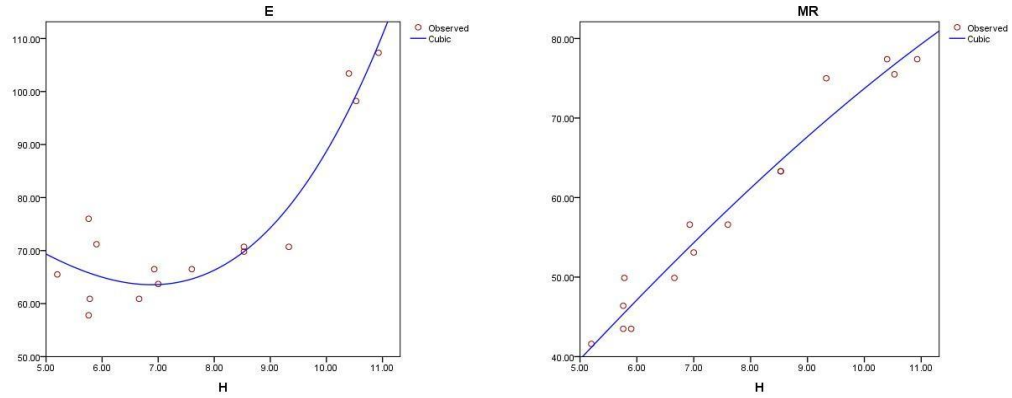

Figure 27: Cubic regression model of E and MR with H(G)

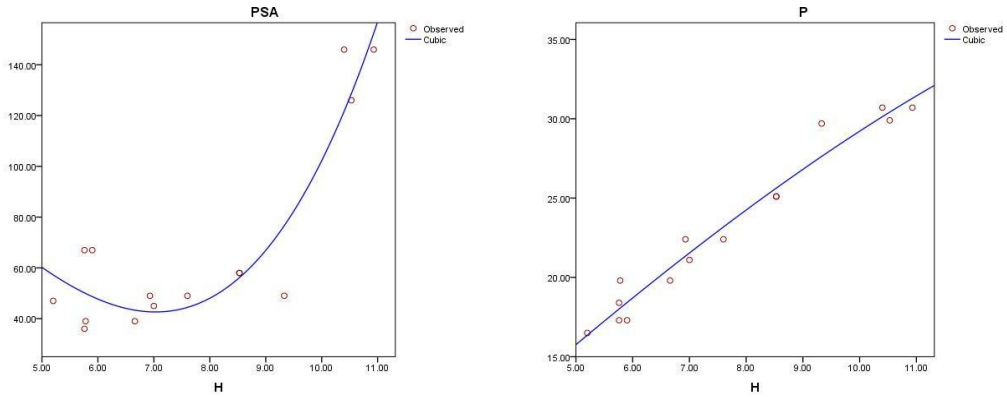

Figure 28: Cubic regression model of PSA and P with $H(G)$

DOI: https://doi.org/10.71058/jodac.v9i6013

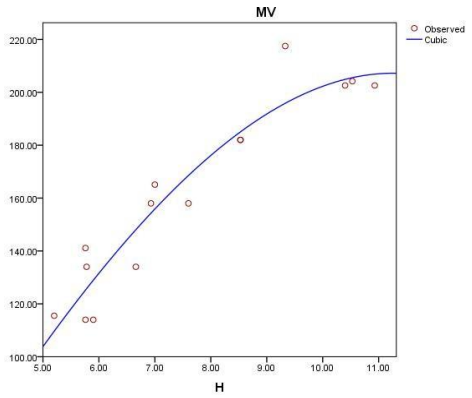

Figure 29: Cubic regression model of MV with *H*(*G*)

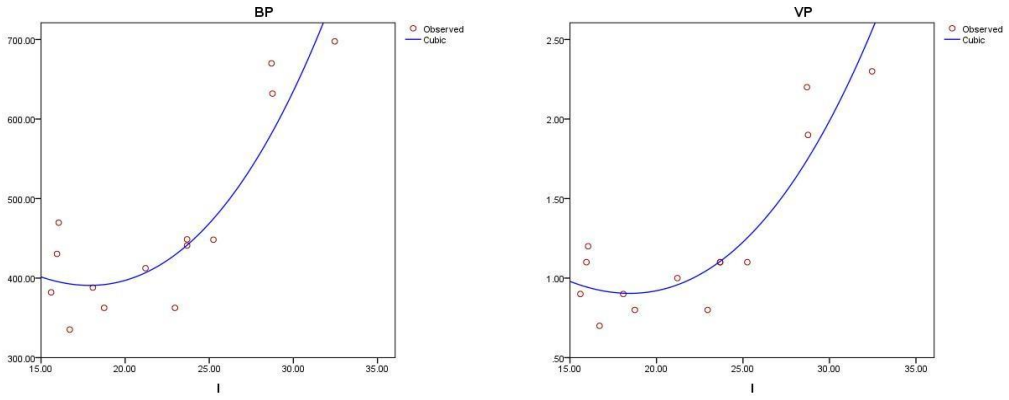

Figure 30: Cubic regression model of BP and VP with *I*(*G*)

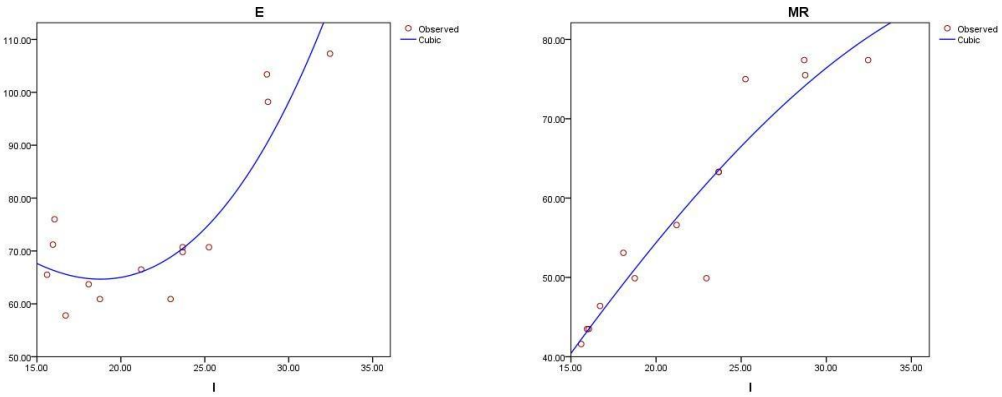

Figure 31: Cubic regression model of E and MR with *I*(*G*)

DOI: https://doi.org/10.71058/jodac.v9i6013

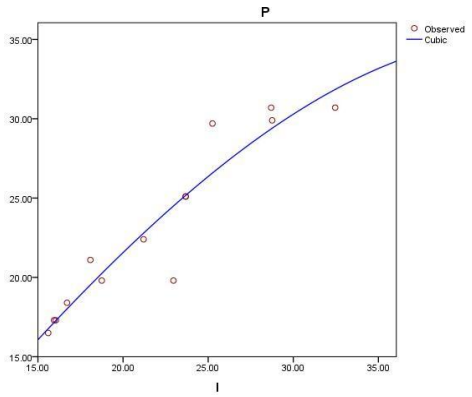

Figure 32: Cubic regression model of P with *I*(*G*)

5.2. 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 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 generalized Randic index, generalized reciprocal Randic index, symmetric division degree index, harmonic index and inverse sum index were considered for the study (see Table 8) with respect to 11 physicochemical properties of coumarins (see Table 7). Among the three regression models we have noticed the following observations:

- For linear regression model, the symmetric division degree index SDD(G), harmonic index H(G) and inverse sum index I(G) shows high predicting power among physicochemical properties of coumarins with correlation coefficient ranging from r=0.900 to r = 0.981 respectively. Further, in all the cases, p = 0.0000 implies that the linear regression model with respect to SDD(G), H(G) and I(G) are highly significant.
- For quadratic regression model the symmetric division degree index SDD(G), harmonic H(G) and inverse sum index I(G) shows high predicting power among physicochemical properties of coumarins with correlation coefficient ranging from r=0.905 to r = 0.982 respectively. Further, in all the cases, p = 0.0000 implies that the linear regression model with respect to SDD(G), H(G) and I(G) are highly significant.
- For cubic regression model, the symmetric division degree index SDD(G), harmonic index H(G) and inverse sum index I(G) shows high predicting power among physicochemical properties of of coumarins with correlation coefficient ranging from r=0.911 to r = 0.982 respectively. Further, in all the cases, p = 0.0000 implies that the linear regression model with respect to SDD(G), H(G) and I(G) are highly significant.

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Conclusion

Coumarins exhibit a wide range of biological activities, such as disease prevention, growth modulation, 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 symmetric division degree index $SDD(G)$, harmonic index $H(G)$ and inverse sum index $I(G)$ are potential topological indices to predict physicochemical properties of coumarins.

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