Evaluating Valency-Based Topological Indices of Polyketide Antibiotics through M-Polynomial Analysis

[1] Priyadharsini G ,Assistant Professor, Department of Mathematics
Kongu Arts and Science College (Autonomous)
Erode,Tamilnadu, India.
[2]Amudhamalar V,Assistant Professor, Department of Mathematics
VET Institute of Arts and Science(Co-ed) College
Erode,Tamilnadu, India.
[3] Savitha S,Assistant Professor, Department of Mathematics
Kongu Arts and Science College (Autonomous)
Erode,Tamilnadu, India.
[4] P.Sathish,Assistant Professor, Department of Mathematics
Nandha Arts and Science College (Autonomous)
Erode,Tamilnadu, India.
[5] S.Shilpa Ivin Emimal,Assistant Professor, Department of Mathematics
St.Theresa's Arts and Science College for Women
Tharangambadi,Tamilnadu, India.

Email: [1]gpmath215@gmail.com , [2]amudhamalarv@gmail.com ,[3] savithamaths85@gmail.com
[4]sathishvishva@gmail.com , [5]shilpaivins@gmail.com

Abstract:

This paper presents an investigation of the structural properties of various short-lived medications utilizing mathematical chemistry methods. The M-polynomial and its complement, are employed to derive and analyze several topological indices and co-indices, such as the first and second Zagreb indices, the F-index, the reformulated Zagreb index, the modified Zagreb index, and the harmonic index. These indices are computed for a set of short-acting medications, including diorcinol, aspilactonol, ascomycotin, aspiketolactonol, aspyronol, engyodontiumone, and lindgomycin. The findings provide valuable insights into the molecular topology and structural characteristics of these pharmaceutical compounds.

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1. Introduction:

The production of massive amounts of biomass in the form of secondary metabolites makes fungi important components of natural environments. Small molecules known as secondary metabolites play no direct role in primary growth, development, reproduction, etc.s. but are essential ecological components that serve as communication, competition, and chemical defenses. From a pharmacological and structural diversity standpoint, polyketides, nonribosomal peptides, alkaloids, and terpenoids are the most significant

and varied classes of fungal secondary metabolites. Polyketides exhibit the widest variety of structural complexity and biological activity, including antimicrobial, anticancer, immune suppressive, and cholesterol-lowering properties. Polyketide synthases (PKS) are large, complex enzymes that biosynthesize polyketides. They produce an amazing amount of chemical scaff by iteratively building carbon backbones from simple acyl-CoA precursors.

Aspergillus and closely related genera (e.g., Engyodontium) stand out for their biosynthetic inventiveness, as they contain many BGCs encoding the enzymes necessary to produce polyketides, such as diorcinol, aspilactonol, ascomycotin, aspiketolactonol, aspyronol and engyodontiumone. This is just one example of the structural and functional diversity present in fungal secondary metabolism.[1-11].

2. Polyketide Biosynthesis:

In fungi, polyketide synthases (PKS), which are large, multi-module proteins, are responsible for producing polyketides. These synthases fall under the category of type I iterative systems. They can also be categorized into three groups based on the degree of reductive processing during chain elongation: highly reducing (HR-PKS), partially reducing (PR-PKS), and non-reducing (NR-PKS) The modular and iterative catalytic mechanisms used by all PKSs include the use of basic building blocks (e.g. A. three more succynyl-CoA); lengthening of chain segments (typically 6–30 carbons); and rises in complexity (e.g., from a simple 5-membered aromatic scaffold to a highly reduced complex polycyclic structure).

Biosynthesis can be conceived as consisting of two steps. First, the assembly of a polyketide chain from the elongation of an acetyl-CoA and malonyl-CoA where the large PKS condenses pn-malonyl-CoA and acetyl-CoA and adds a polyketide moiety. The growing chain will then be further elaborated via a series of tailoring reactions e.g., oxidative, methylation, reductive, halogenation, cyclization where these introduce additional functional groups and compound complexity. Polyketides produced can have varying levels of biological activity; this makes them highly valuable platforms for the development of new medicines and other biotechnological pharmaceutical products.[1-11]

3 .Materials and Methods:

3.1Diorcinol:

Diorcinol is a phenolic polyketide generated in a variety of Aspergillus species, displaying a wide distribution among A. sydowii, A. flocculus, and A. versicolor, and in other endophytic fungi. Diorcinol is formed by a non-reducing PKS (NRPKS) that produces the polyketide dimer of diphenyl ether, which is diorcinol's core skeleton. Biosynthesis of diorcinol occurs via an NRPKS coded by the gene AspksD (similar to A. nidulans AN7909), which assembles the polyketide backbone; the NRPKS is followed by two unspecified decarboxylating enzymes (AN7910 and AN7911), which together yield diorcinol.

Diorcinol production is regulated by environmental conditions that can promote biosynthetic gene expression and improve metabolite yield in deep-sea and marine-derived fungus, such as high hydrostatic pressure. This highlights the adaptive relationship between fungal metabolism and environmental stress, as well as how the ecological context influences the biosynthesis and bioactivity of fungal secondary metabolites..[12-17]

3.2. Aspilactonol:

Aspilactnol is a polyketide metabolite found in marine fungal isolates, such as Aspergillus species like A versicolor (Li and others) which binds to other bioactive polyketides, has a macrolactone ring that resembles those in other polyketides. A highly reducing PKS most likely biosynthesizes the polyketide, and aspilactonol is formed by enzymatic cyclization of the lactone moiety. [12-17]

3.3Ascomycotin:

Ascomycotin is a bicyclic polyketide isolated from some of the Ascomycota and is likely produced by a PKS with cyclization and oxidation at the biogenesis stage. It features a fused bicyclic core with hydroxyl and methyl groups placed after the original assembly by tailoring enzymes, it also has a number of other functional groups that give a range of biological activity, but these have yet to be ciphered regarding bioactivity. Ascomycotin's basic structure and functional groups alone nominate it for future research. .[12-17]

3.4 Aspiketolactonol:

As isolated from marine-derived fungi, aspiketolactonol also contains a lactone ring, a structural motif likely biosynthesized by a polyketide synthase (PKS) that produces a polyketide backbone, followed by the full cyclization to yield the lactone motif .Lactones, such as aspiketolactonol, can have advantageous implications with respect to biological activity because they can be more biologically soluble and faster to bind onto targeted

biological or chemical target(s). The biosynthesis pathway for aspiketolactonol elucidates the phenotypic flexibility of these fungal PKSs into new ecological niches such as the marine environments where they could in turn produce specialized metabolites to acquire competitive advantages.

[12-17]

3.5 Aspyronol:

Aspyronol is a polyketide derived from Aspergillus species that, like other polyketides, is biosynthesized using a PKS with additional modifications to produce the final compound. These modifications can include methylation, oxidation, or any number of tailoring reactions that can add more functional groups, and for example improve the bioactivity of the compound. The fact that aspyronol is a structurally diverse polyketide is due to the modular and iterative characteristics of fungal PKSs, which are capable of adding different starter and extender units, and reduce, dehydrating, and methylate portions during the biosynthesis..[12-17]

3.6Engyodontiumone:

Engyodontiumone is a polyketide from the aquatic fungus Engyodontium album with a structure that serves as a typical example of polyketide-derived bicyclic core structures with different numbers of hydroxyl and methyl groups. The enzymology of engyodontiumone biosynthesis is based on a type I PKS that assembles the skeleton followed by cyclization followed by oxidative tailoring. Engyodontiumone and congeners have many different biological activities, including antibiotic and cytotoxic properties, demonstrating the drug potential of marine fungi metabolites.[12-17]

4. Preliminaries:

Let $\Omega = (V, E)$ be a graph where V and E represented the vertex and edge set respectively. In molecular graph the vertices and edges represented the atoms and chemical bonds. The degree of a vertex is the number of edges incident to u and it is denoted by d_u.Order denotes the number of vertices present in the graph and size denotes the number of edges present in the graph.

M – Polynomial: [19-26]

M – polynomial of a graph Ω denoted as $\mathcal{M}(\Omega; a, b)$ is $\mathcal{M}(\Omega; a, b) = \sum_{e \in E} m_{r,s}(\Omega) a^r b^s$

Where $m_{r,s}$ is denoted as edge partition.

Table:1 Derivation of DBTI from $\mathcal{M}$ – Polynomial: [19-26]

$TI's$	$Derivation\ \ from\ M(W,a,b)$
M_1	$(D_a + D_b)g(a,b)\|_{a=b=1}$
M_2	$(D_a D_b)g(a,b)\|_{a=b=1}$
F	$(D^2{}_a + D^2{}_b)g(a,b)\|_{a=b=1}$
RZ_3	$D_a D_b (D_a + D_b)g(a,b)\|_{a=b=1}$
MM_2	$T_a T_b g(a,b)\|_{a=b=1}$
H	$(2T_a J)g(a,b)\|_{a=b=1}$

$\bar{M}$ -Polynomial: [27]

$\bar{M}$– polynomial of a graph Ω denoted as $\bar{M}(\Omega; a, b)$ is

$$\bar{M}(\Omega; a, b) = \sum_{e \notin E} \bar{m}_{r,s}(\Omega) a^r b^s$$

Table:2 Derivation of DBTCI from $\bar{M}$ – Polynomial: [27]

$TI's$	$Derivation\ \ from\ \overline{M}(W,a,b)$
$\overline{M}_1$	$(c_a + c_b)g(a,b)\|_{a=b=1}$
$\overline{M}_2$	$(c_a c_b)g(a,b)\|_{a=b=1}$
$\overline{F}$	$(c^2{}_a + c^2{}_b)g(a,b)\|_{a=b=1}$
$\overline{RZ}_3$	$c_a c_b (c_a + c_b)g(a,b)\|_{a=b=1}$
$\overline{MM}_2$	$T_a T_b g(a,b)\|_{a=b=1}$
$\overline{H}$	$(2T_a J)g(a,b)\|_{a=b=1}$

$$r = s \Rightarrow \overline{m}_{rs} = \frac{s_r (s_r - 1)}{2} - m_{rr}$$

$$r < s \Rightarrow \overline{m}_{rs} = s_r s_s - m_{rs}$$

4.1 Main Results:

In this section, we present the results for the $\mathcal{M}$ – polynomial and the $\bar{M}$ -polynomial of the molecular graphs corresponding to secondary metabolites of polyketides derived from deep-sea fungus, computed using degree based and valency-based indices.

Theorem: 4.1.1

Let Ω denote the molecular graph of aspilactonol. Then, the $\mathcal{M}$ – polynomial and the $\bar{M}$ -polynomial polynomial for Ω are given by:

1. M – polynomial for Ω is
$$M(\Omega; a, b) = 3ab^3 + 2ab^4 + 4a^2b^3 + 2a^2b^4 + a^2b^2 + a^3b^3$$
2. $\bar{M}$ -polynomial for Ω is
$$\bar{M}(\Omega; a, b) = 12ab^3 + 3ab^4 + 8a^2b^3 + 2a^2b^4 + 5a^2b^2 + 2a^3b^3$$

Proposition: 4.1.2

Let Ω be the molecular graph of Aspilactonol. Then

M – polynomial	$\bar{M}$ -polynomial
1. $M_1(\Omega) = 64$	1. $\bar{M}_1(\Omega) = 147$
2. $M_2(\Omega) = 70$	2. $\bar{M}_2(\Omega) = 148$
3. $F(\Omega) = 182$	3.$\bar{F}(\Omega) = 389$
4. $RZ_3(\Omega) = 362$	4. $\overline{RZ}_3(\Omega) = 728$
5.$MM_2(\Omega) = \frac{115}{36}$	5.$\overline{MM_2}(\Omega) = \frac{136}{36}$
6.$H(\Omega) = \frac{27}{5}$	6.$\bar{H}(\Omega) = \frac{360}{15}$

Proof: Part:1

$M(\Omega; a, b) = g(a, b) = 3ab^3 + 2ab^4 + 4a^2b^3 + 2a^2b^4 + a^2b^2 + a^3b^3$

$\Delta_a g(a, b) = 3ab^3 + 2ab^4 + 8a^2b^3 + 4a^2b^4 + 2a^2b^2 + 3a^3b^3$

$\Delta_b g(a, b) = 9ab^3 + 8ab^4 + 12a^2b^3 + 8a^2b^4 + 2a^2b^2 + 3a^3b^3$

$(\Delta_a + \Delta_b)g(a, b) = 12ab^3 + 10ab^4 + 20a^2b^3 + 12a^2b^4 + 4a^2b^2 + 6a^3b^3$

$(\Delta_b\Delta_a)g(a, b) = 9ab^3 + 8ab^4 + 24a^2b^3 + 16a^2b^4 + 4a^2b^2 + 9a^3b^3$

$(\Delta_a^2 + \Delta_b^2)g(a, b) = 30ab^3 + 34ab^4 + 52a^2b^3 + 40a^2b^4 + 8a^2b^2 + 18a^3b^3$

$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a, b) = 36ab^3 + 40ab^4 + 120a^2b^3 + 96a^2b^4 + 16a^2b^2 + 54a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = ab^3 + \frac{1}{2}ab^4 + 2a^2b^3 + \frac{1}{4}a^2b^4 + \frac{1}{4}a^2b^2 + \frac{1}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = 2a^4 + \frac{12}{5}a^5 + a^6$

Part:2

$\bar{M}(\Omega; a, b) = g(a, b) = 12ab^3 + 3ab^4 + 8a^2b^3 + 2a^2b^4 + 5a^2b^2 + 2a^3b^3$

$\chi_a g(a, b) = 12ab^3 + 3ab^4 + 16a^2b^3 + 4a^2b^4 + 10a^2b^2 + 6a^3b^3$

$\chi_b g(a, b) = 36ab^3 + 12ab^4 + 24a^2b^3 + 8a^2b^4 + 10a^2b^2 + 6a^3b^3$

$(\chi_a + \chi_b)g(a, b) = 48ab^3 + 15ab^4 + 40a^2b^3 + 12a^2b^4 + 20a^2b^2 + 12a^3b^3$

$(\chi_a\chi_b)g(a, b) = 36ab^3 + 12ab^4 + 48a^2b^3 + 16a^2b^4 + 20a^2b^2 + 12a^3b^3$

$(\chi_a^2 + \chi_b^2)g(a, b) = 120ab^3 + 51ab^4 + 102a^2b^3 + 40a^2b^4 + 40a^2b^2 + 36a^3b^3$

$\chi_a\chi_b(\chi_a + \chi_b)g(a, b) = 144ab^3 + 60ab^4 + 240a^2b^3 + 96a^2b^4 + 80a^2b^2 + 108a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = 4ab^3 + \frac{3}{4}ab^4 + \frac{4}{3}a^2b^3 + \frac{1}{4}a^2b^4 + \frac{5}{4}a^2b^2 + \frac{2}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = \frac{11}{5}a^5 + \frac{4}{3}a^6 + \frac{17}{2}a^4$

Theorem: 4.1.3

Let Ω be the molecular graph of Aspyronol. Then the

1. M – polynomial for Ω is
$$M(\Omega; a, b) = 2ab^2 + 6a^2b^3 + 3ab^3 + 3a^3b^3$$
2. $\bar{M}$ -polynomial for Ω is
$$\bar{M}(\Omega; a, b) = 18ab^2 + 22ab^3 + 14a^2b^3 + 7a^3b^3$$

Proposition:4.1.4

Let Ω be the molecular graph of Aspyronol. Then

M – polynomial	$\bar{M}$ -polynomial

1. $M_1(\Omega) = 66$	1. $\overline{M}_1(\Omega) = 254$
2. $M_2(\Omega) = 76$	2. $\overline{M}_2(\Omega) = 249$
3. $F(\Omega) = 172$	3. $\overline{F}(\Omega) = 618$
4. $RZ_3(\Omega) = 390$	4. $\overline{RZ}_3(\Omega) = 829$
5. $MM_2(\Omega) = \frac{10}{3}$	5. $\overline{MM_2}(\Omega) = \frac{284}{18}$
6. $H(\Omega) = \frac{187}{30}$	6. $\overline{H}(\Omega) = \frac{464}{15}$

Proof: Part:1

$M(\Omega; a, b) = g(a, b) = 2ab^2 + 6a^2b^3 + 3ab^3 + 3a^3b^3$

$\Delta_a g(a, b) = 2ab^2 + 12a^2b^3 + 3ab^3 + 9a^3b^3$

$\Delta_b g(a, b) = 4ab^2 + 18a^2b^3 + 9ab^3 + 9a^3b^3$

$(\Delta_a + \Delta_b)g(a, b) = 6ab^2 + 30a^2b^3 + 12ab^3 + 18a^3b^3$

$(\Delta_b\Delta_a)g(a, b) = 4ab^2 + 36a^2b^3 + 27ab^3 + 9a^3b^3$

$(\Delta_a^2 + \Delta_b^2)g(a, b) = 10ab^2 + 78a^2b^3 + 54ab^3 + 30a^3b^3$

$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a, b) = 12ab^2 + 180a^2b^3 + 36ab^3 + 162a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = ab^2 + a^2b^3 + ab^3 + \frac{1}{3}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = a^6 + \frac{4}{3}a^3 + \frac{12}{5}a^5 + \frac{3}{2}a^4$

Part:2

$\overline{M}(\Omega; a, b) = g(a, b) = 18ab^2 + 22ab^3 + 14a^2b^3 + 7a^3b^3$

$\chi_a g(a, b) = 18ab^2 + 22ab^3 + 28a^2b^3 + 21a^3b^3$

$\chi_b g(a, b) = 18ab^2 + 66ab^3 + 42a^2b^3 + 21a^3b^3$

$(\chi_a + \chi_b)g(a, b) = 54ab^2 + 88ab^3 + 70a^2b^3 + 42a^3b^3$

$(\chi_a\chi_b)g(a, b) = 36ab^2 + 66ab^3 + 84a^2b^3 + 63a^3b^3$

$(\chi_a^2 + \chi_b^2)g(a, b) = 90ab^2 + 220ab^3 + 182a^2b^3 + 126a^3b^3$

$\chi_a\chi_b(\chi_a + \chi_b)g(a, b) = 108ab^2 + 264ab^3 + 420a^2b^3 + 37a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = 9ab^2 + \frac{22}{3}ab^3 + \frac{14}{6}a^2b^3 + \frac{7}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = 12a^3 + 11a^4 + \frac{28}{5}a^5 + \frac{7}{3}a^6$

Theorem: 4.1.5

Let Ω be the molecular graph of Ascomycotin. Then the

1. M – polynomial for Ω is
$$M(\Omega; a, b) = 6ab^3 + 8a^2b^3 + a^2b^2 + 8a^3b^3$$
2. $\overline{M}$ -polynomial for Ω is
$$\overline{M}(\Omega; a, b) = 54ab^3 + 42a^2b^3 + 9a^2b^2 + 38a^3b^3$$

Proposition:4.1.6

Let Ω be the molecular graph of Ascomycotin. Then

M – polynomial	$\overline{M}$ -polynomial

1. $M_1(\Omega) = 116$	1. $\bar{M}_1(\Omega) = 690$
2. $M_2(\Omega) = 142$	2. $\bar{M}_2(\Omega) = 792$
3. $F(\Omega) = 316$	3.$\bar{F}(\Omega) = 1842$
4. $RZ_3(\Omega) = 760$	4. $\overline{RZ}_3(\Omega) = 3420$
5.$MM_2(\Omega) = \frac{161}{36}$	5.$\overline{MM_2}(\Omega) = \frac{607}{18}$
6.$H(\Omega) = \frac{281}{30}$	6.$\bar{H}(\Omega) = \frac{1829}{30}$

Proof: Part:1

$M(\Omega; a, b) = g(a, b) = 6ab^3 + 8a^2b^3 + a^2b^2 + 8a^3b^3$

$\Delta_a g(a, b) = 6ab^3 + 16a^2b^3 + a^2b^2 + 24a^3b^3$

$\Delta_b g(a, b) = 18ab^3 + 24a^2b^3 + 2a^2b^2 + 24a^3b^3$

$(\Delta_a + \Delta_b)g(a, b) = 24ab^3 + 40a^2b^3 + 4a^2b^2 + 48a^3b^3$

$(\Delta_b\Delta_a)g(a, b) = 18ab^3 + 48a^2b^3 + 4a^2b^2 + 72a^3b^3$

$(\Delta_a^2 + \Delta_b^2)g(a, b) = 60ab^3 + 104a^2b^3 + 8a^2b^2 + 144a^3b^3$

$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a, b) = 72ab^3 + 240a^2b^3 + 16a^2b^2 + 432a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = 2ab^3 + \frac{4}{3}a^2b^3 + \frac{1}{4}a^2b^2 + \frac{8}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = 3a^4 + \frac{16}{5}a^5 + \frac{8}{3}a^6 + \frac{1}{2}a^4$

Part:2

$\bar{M}(\Omega; a, b) = g(a, b) = 54ab^3 + 42a^2b^3 + 9a^2b^2 + 38a^3b^3$

$\chi_a g(a, b) = 54ab^3 + 84a^2b^3 + 18a^2b^2 + 114a^3b^3$

$\chi_b g(a, b) = 162ab^3 + 126a^2b^3 + 18a^2b^2 + 114a^3b^3$

$(\chi_a + \chi_b)g(a, b) = 216ab^3 + 210a^2b^3 + 36a^2b^2 + 228a^3b^3$

$(\chi_a\chi_b)g(a, b) = 162ab^3 + 252a^2b^3 + 36a^2b^2 + 342a^3b^3$

$(\chi_a^2 + \chi_b^2)g(a, b) = 540ab^3 + 546a^2b^3 + 72a^2b^2 + 684a^3b^3$

$\chi_a\chi_b(\chi_a + \chi_b)g(a, b) = 648ab^3 + 1260a^2b^3 + 144a^2b^2 + 1368a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = \frac{54}{3}ab^3 + \frac{42}{6}a^2b^3 + \frac{9}{2}a^2b^2 + \frac{38}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = \frac{126}{4}a^4 + \frac{84}{5}a^5 + \frac{76}{6}a^6$

Theorem: 4.1.7

Let Ω be the molecular graph of Diorcinol. Then the

1. M – polynomial for Ω is
$$M(\Omega; a, b) = 4ab^3 + 14a^2b^3$$
2. $\bar{M}$ -polynomial for Ω is
$$\bar{M}(\Omega; a, b) = 20ab^3 + 28a^2b^3$$

Proposition: 4.1.8

Let Ω be the molecular graph of Diorcinol. Then

M – polynomial	$\bar{M}$ -polynomial

1. $M_1(\Omega) = 86$ 2. $M_2(\Omega) = 96$ 3. $F(\Omega) = 222$ 4. $RZ_3(\Omega) = 468$ 5.$MM_2(\Omega) = 6$ 6.$H(\Omega) = \frac{38}{5}$	1. $\overline{M}_1(\Omega) = 220$ 2. $\overline{M}_2(\Omega) = 222$ 3.$\overline{F}(\Omega) = 564$ 4. $\overline{RZ}_3(\Omega) = 1080$ 5.$\overline{MM_2}(\Omega) = \frac{68}{6}$ 6.$\overline{H}(\Omega) = \frac{106}{5}$

Proof: Part:1

$M(\Omega; a, b) = g(a, b) = 4ab^3 + 14a^2b^3$

$\Delta_a g(a, b) = 4ab^3 + 28a^2b^3$

$\Delta_b g(a, b) = 12ab^3 + 42a^2b^3$

$(\Delta_a + \Delta_b)g(a, b) = 16ab^3 + 70a^2b^3$

$(\Delta_b\Delta_a)g(a, b) = 12ab^3 + 84a^2b^3$

$(\Delta_a^2 + \Delta_b^2)g(a, b) = 40ab^3 + 182a^2b^3$

$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a, b) = 48ab^3 + 420a^2b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = \frac{4}{3}ab^3 + \frac{14}{3}a^2b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = 2a^4 + \frac{28}{5}a^5$

Part:2

$\overline{M}(\Omega; a, b) = g(a, b) = 20ab^3 + 28a^2b^3$

$\chi_a g(a, b) = 20ab^3 + 56a^2b^3$

$\chi_b g(a, b) = 60ab^3 + 84a^2b^3$

$(\chi_a + \chi_b)g(a, b) = 80ab^3 + 140a^2b^3$

$(\chi_a\chi_b)g(a, b) = 60ab^3 + 162a^2b^3$

$(\chi_a^2 + \chi_b^2)g(a, b) = 200ab^3 + 364a^2b^3$

$\chi_a\chi_b(\chi_a + \chi_b)g(a, b) = 240ab^3 + 840a^2b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = \frac{20}{3}ab^3 + \frac{28}{6}a^2b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = 10a^4 + \frac{56}{5}a^5$

Theorem: 4.1.9

Let Ω be the molecular graph of Aspiketolactonol. Then the

1. M – polynomial for Ω is
$$M(\Omega; a, b) = 4ab^4 + 3ab^3 + 4a^2b^3 + 2a^2b^4 + a^4b^4 + a^3b^3$$
2. $\overline{M}$ -polynomial for Ω is
$$\overline{M}(\Omega; a, b) = 10ab^4 + 18ab^3 + 5a^2b^3 + 4a^2b^4 + 2a^3b^3$$

Proposition:4.1.10

Let Ω be the molecular graph of Aspiketolactonol. Then

M – polynomial	$\overline{M}$ -polynomial

1. $M_1(\Omega) = 78$	1. $\bar{M}_1(\Omega) = 183$
2. $M_2(\Omega) = 70$	2. $\bar{M}_2(\Omega) = 174$
3. $F(\Omega) = 240$	3. $\bar{F}(\Omega) = 515$
4. $RZ_3(\Omega) = 514$	4. $\overline{RZ}_3(\Omega) = 866$
5. $MM_2(\Omega) = \frac{59}{18}$	5. $\overline{MM_2}(\Omega) = \frac{181}{18}$
6. $H(\Omega) = \frac{63}{20}$	6. $\bar{H}(\Omega) = 17$

Proof:Part:1

$M(\Omega; a, b) = g(a, b) = 4ab^4 + 3ab^3 + 4a^2b^3 + 2a^2b^4 + a^4b^4 + a^3b^3$

$\Delta_a g(a, b) = 4ab^4 + 3ab^3 + 8a^2b^3 + 4a^2b^4 + 4a^4b^4 + 3a^3b^3$

$\Delta_b g(a, b) = 16ab^4 + 9ab^3 + 12a^2b^3 + 8a^2b^4 + 4a^4b^4 + 3a^3b^3$

$(\Delta_a + \Delta_b)g(a, b) = 20ab^4 + 12ab^3 + 20a^2b^3 + 12a^2b^4 + 8a^4b^4 + 6a^3b^3$

$(\Delta_b\Delta_a)g(a, b) = 16ab^4 + 9ab^3 + 24a^2b^3 + 16a^2b^4 + 16a^4b^4 + 9a^3b^3$

$(\Delta_a^2 + \Delta_b^2)g(a, b) = 68ab^4 + 30ab^3 + 52a^2b^3 + 40a^2b^4 + 32a^4b^4 + 18a^3b^3$

$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a, b) = 80ab^4 + 36ab^3 + 120a^2b^3 + 96a^2b^4 + 128a^4b^4 + 54a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = ab^4 + ab^3 + \frac{2}{3}a^2b^3 + \frac{1}{4}a^2b^4 + \frac{1}{4}a^4b^4 + \frac{1}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = a^6 + \frac{2}{5}a^5 + \frac{1}{4}a^8 + \frac{3}{2}a^4$

Part:2

$\bar{M}(\Omega; a, b) = g(a, b) = 10ab^4 + 18ab^3 + 5a^2b^3 + 4a^2b^4 + 2a^3b^3$

$\chi_a g(a, b) = 10ab^4 + 18ab^3 + 10a^2b^3 + 8a^2b^4 + 6a^3b^3$

$\chi_b g(a, b) = 40ab^4 + 54ab^3 + 15a^2b^3 + 16a^2b^4 + 6a^3b^3$

$(\chi_a + \chi_b)g(a, b) = 50ab^4 + 72ab^3 + 25a^2b^3 + 24a^2b^4 + 12a^3b^3$

$(\chi_a\chi_b)g(a, b) = 40ab^4 + 54ab^3 + 30a^2b^3 + 32a^2b^4 + 18a^3b^3$

$(\chi_a^2 + \chi_b^2)g(a, b) = 170ab^4 + 180ab^3 + 65a^2b^3 + 64a^2b^4 + 36a^3b^3$

$\chi_a\chi_b(\chi_a + \chi_b)g(a, b) = 216ab^3 + 200ab^4 + 150a^2b^3 + 192a^2b^4 + 108a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = \frac{5}{2}ab^4 + 6ab^3 + \frac{5}{6}a^2b^3 + \frac{1}{2}a^2b^4 + \frac{2}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = 9a^4 + 6a^5 + 2a^6$

Theorem: 4.1.11

Let Ω be the molecular graph of Engyodontiumone. Then the

1. M – polynomial for Ω is
$$M(\Omega; a, b) = 2ab^2 + 5ab^3 + 10a^2b^3 + 9a^3b^3$$
2. $\bar{M}$ -polynomial for Ω is
$$\bar{M}(\Omega; a, b) = 40ab^2 + 72ab^3 + 56a^2b^3 + 44a^3b^3$$

Proposition:4.1.12

Let Ω be the molecular graph of Engyodontiumone. Then

M – polynomial	$\bar{M}$ -polynomial

1. $M_1(\Omega) = 130$	1. $\bar{M}_1(\Omega) = 952$
2. $M_2(\Omega) = 160$	2. $\bar{M}_2(\Omega) = 1028$
3. $F(\Omega) = 352$	3.$\bar{F}(\Omega) = 2440$
4. $RZ_3(\Omega) = 858$	4. $\overline{RZ}_3(\Omega) = 5160$
5.$MM_2(\Omega) = \frac{16}{3}$	5.$\overline{MM_2}(\Omega) = \frac{172}{9}$
6.$H(\Omega) = \frac{53}{6}$	6.$\bar{H}(\Omega) = \frac{1832}{15}$

Proof: Part:1

$M(\Omega; a, b) = g(a, b) = 2ab^2 + 5ab^3 + 10a^2b^3 + 9a^3b^3$

$\Delta_a g(a, b) = 2ab^2 + 5ab^3 + 20a^2b^3 + 27a^3b^3$

$\Delta_b g(a, b) = 4ab^2 + 15ab^3 + 30a^2b^3 + 27a^3b^3$

$(\Delta_a + \Delta_b)g(a, b) = 6ab^2 + 20ab^3 + 50a^2b^3 + 54a^3b^3$

$(\Delta_b\Delta_a)g(a, b) = 4ab^2 + 15ab^3 + 60a^2b^3 + 81a^3b^3$

$(\Delta_a^2 + \Delta_b^2)g(a, b) = 10ab^2 + 50ab^3 + 130a^2b^3 + 162a^3b^3$

$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a, b) = 12ab^2 + 60ab^3 + 300a^2b^3 + 486a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = ab^2 + \frac{5}{3}ab^3 + \frac{5}{3}a^2b^3 + a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = \frac{4}{3}a^3 + 4a^5 + \frac{5}{2}a^4 + 3a^6$

Part:2

$\bar{M}(\Omega; a, b) = g(a, b) = 40ab^2 + 72ab^3 + 56a^2b^3 + 44a^3b^3$

$\chi_a g(a, b) = 40ab^2 + 72ab^3 + 112a^2b^3 + 132a^3b^3$

$\chi_b g(a, b) = 80ab^2 + 216ab^3 + 168a^2b^3 + 132a^3b^3$

$(\chi_a + \chi_b)g(a, b) = 120ab^2 + 288ab^3 + 280a^2b^3 + 264a^3b^3$

$(\chi_a\chi_b)g(a, b) = 80ab^2 + 216ab^3 + 336a^2b^3 + 396a^3b^3$

$(\chi_a^2 + \chi_b^2)g(a, b) = 200ab^2 + 720ab^3 + 728a^2b^3 + 792a^3b^3$

$\chi_a\chi_b(\chi_a + \chi_b)g(a, b) = 240ab^2 + 864ab^3 + 1680a^2b^3 + 2376a^3b^3$

$\mathrm{T}_a\mathrm{T}_b g(a, b) = 20ab^2 + 24ab^3 + \frac{28}{3}a^2b^3 + \frac{44}{9}a^3b^3$

$2(\mathrm{T}_a\mathrm{I})g(a, b) = \frac{80}{3}a^3 + 36a^4 + \frac{224}{5}a^5 + \frac{44}{3}a^6$

Theorem: 4.1.13

Let Ω be the molecular graph of Lindgomycin. Then the

1. M – polynomial for Ω is
   $M(\Omega; a, b) = ab^2 + 9a^2b^2 + 3ab^3 + 8a^2b^3 + 6a^3b^3 + 2ab^4 + 4a^2b^4 + a^4b^4$
2. $\bar{M}$ -polynomial for Ω is
   $\bar{M}(\Omega; a, b) = 89ab^2 + 96a^2b^2 + 45ab^3 + 112a^2b^3 + 22a^3b^3 + 10ab^4 + 26a^2b^4$

Proposition: 4.1.14

Let Ω be the molecular graph of Lindgomycin. Then

M – polynomial	$\bar{M}$ -polynomial

1. $M_1(\Omega) = 169$	1. $\bar{M}_1(\Omega) = 1549$
2. $M_2(\Omega) = 205$	2. $\bar{M}_2(\Omega) = 1635$
3. $F(\Omega) = 445$	3.$\bar{F}(\Omega) = 3845$
4. $RZ_3(\Omega) = 1136$	4. $\overline{RZ}_3(\Omega) = 7886$
5.$MM_2(\Omega) = \frac{327}{48}$	5.$\overline{MM_2}(\Omega) = \frac{3973}{36}$
6.$H(\Omega) = \frac{177}{4}$	6.$\bar{H}(\Omega) = \frac{5839}{30}$

Proof:Part:1

$$M(\Omega;a,b) = g(a,b) = ab^2 + 9a^2b^2 + 3ab^3 + 8a^2b^3 + 6a^3b^3 + 2ab^4 + 4a^2b^4 + a^4b^4$$

$$\Delta_a g(a,b) = ab^2 + 18a^2b^2 + 3ab^3 + 16a^2b^3 + 18a^3b^3 + 2ab^4 + 8a^2b^4 + 4a^4b^4$$

$$\Delta_b g(a,b) = 2ab^2 + 18a^2b^2 + 9ab^3 + 24a^2b^3 + 18a^3b^3 + 8ab^4 + 16a^2b^4 + 4a^4b^4$$

$$(\Delta_a + \Delta_b)g(a,b) = 3ab^2 + 36a^2b^2 + 12ab^3 + 40a^2b^3 + 36a^3b^3 + 10ab^4 + 24a^2b^4 + 8a^4b^4$$

$$(\Delta_b\Delta_a)g(a,b) = 2ab^2 + 36a^2b^2 + 9ab^3 + 48a^2b^3 + 54a^3b^3 + 8ab^4 + 32a^2b^4 + 16a^4b^4$$

$$(\Delta_a^2 + \Delta_b^2)g(a,b) = 5ab^2 + 72a^2b^2 + 30ab^3 + 104a^2b^3 + 108a^3b^3 + 34ab^4 + 80a^2b^4 + 32a^4b^4$$

$$\Delta_a\Delta_b(\Delta_a + \Delta_b)g(a,b) = 32ab^2 + 144a^2b^2 + 36ab^3 + 240a^2b^3 + 324a^3b^3 + 40ab^4 + 192a^2b^4 + 128a^4b^4$$

$$\mathrm{T}_a\mathrm{T}_b g(a,b) = \frac{1}{2}ab^2 + \frac{9}{4}a^2b^2 + ab^3 + \frac{4}{3}a^2b^3 + \frac{2}{3}a^3b^3 + \frac{1}{2}ab^4 + \frac{1}{2}a^2b^4 + \frac{1}{16}a^4b^4$$

$$2(\mathrm{T}_a\mathrm{I})g(a,b) = \frac{2}{3}a^3 + 36a^4 + 4a^5 + \frac{10}{3}a^6 + \frac{1}{4}a^8$$

Part:2

$$\bar{M}(\Omega;a,b) = g(a,b) = 89ab^2 + 96a^2b^2 + 45ab^3 + 112a^2b^3 + 22a^3b^3 + 10ab^4 + 26a^2b^4$$

$$\chi_a g(a,b) = 89ab^2 + 102a^2b^2 + 45ab^3 + 224a^2b^3 + 66a^3b^3 + 10ab^4 + 52a^2b^4$$

$$\chi_b g(a,b) = 178ab^2 + 102a^2b^2 + 125ab^3 + 336a^2b^3 + 66a^3b^3 + 40ab^4 + 104a^2b^4$$

$$(\chi_a + \chi_b)g(a,b) = 267ab^2 + 204a^2b^2 + 180ab^3 + 560a^2b^3 + 132a^3b^3 + 50ab^4 + 156a^2b^4$$

$$(\chi_a\chi_b)g(a,b) = 178ab^2 + 204a^2b^2 + 135ab^3 + 672a^2b^3 + 198a^3b^3 + 40ab^4 + 208a^2b^4$$

$$(\chi_a^2 + \chi_b^2)g(a,b) = 445ab^2 + 408a^2b^2 + 450ab^3 + 1456a^2b^3 + 396a^3b^3 + 170ab^4 + 520a^2b^4$$

$$\chi_a\chi_b(\chi_a + \chi_b)g(a,b) = 534ab^2 + 816a^2b^2 + 540ab^3 + 3360a^2b^3 + 1188a^3b^3 + 200ab^4 + 1248a^2b^4$$

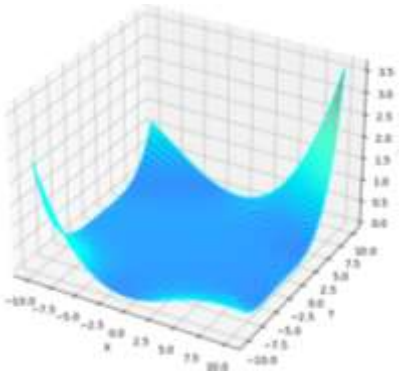
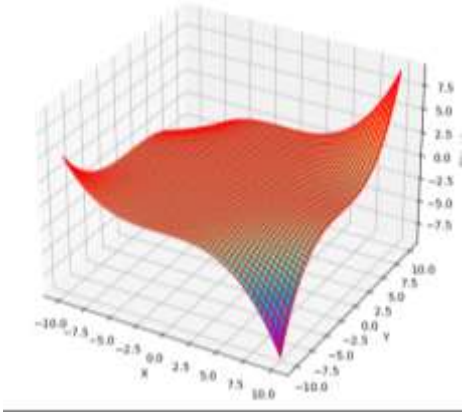
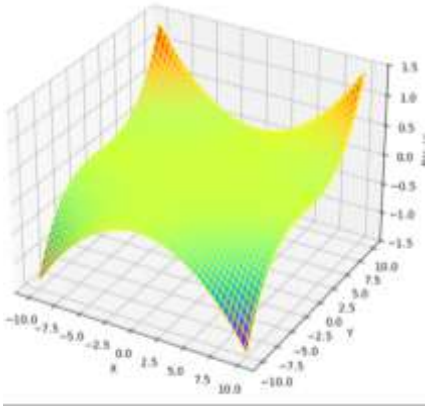
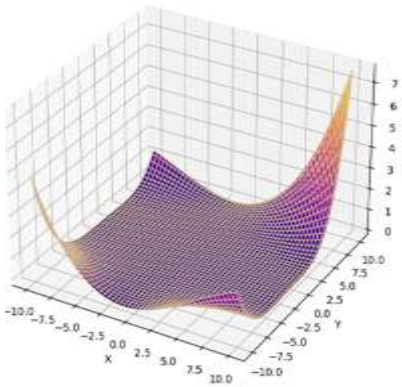
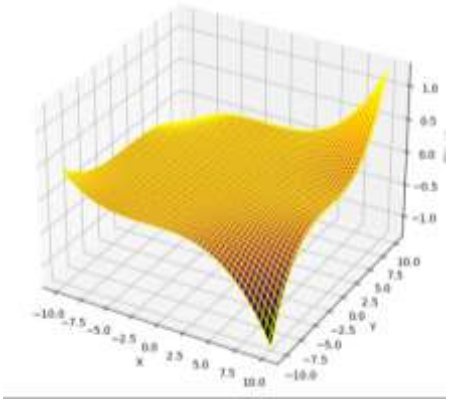
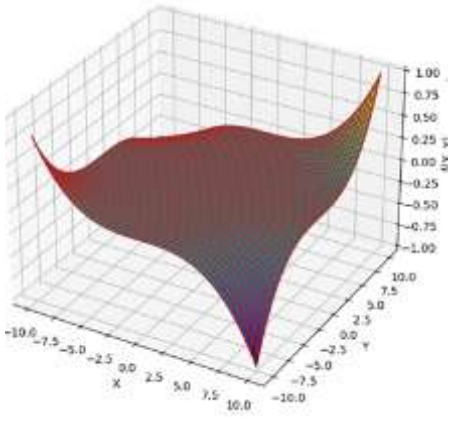
$$\mathrm{T}_a\mathrm{T}_b g(a,b) = \frac{89}{2}ab^2 + 24a^2b^2 + 15ab^3 + \frac{56}{3}a^2b^3 + \frac{22}{9}a^3b^3 + \frac{5}{2}ab^4 + \frac{13}{4}a^2b^4$$

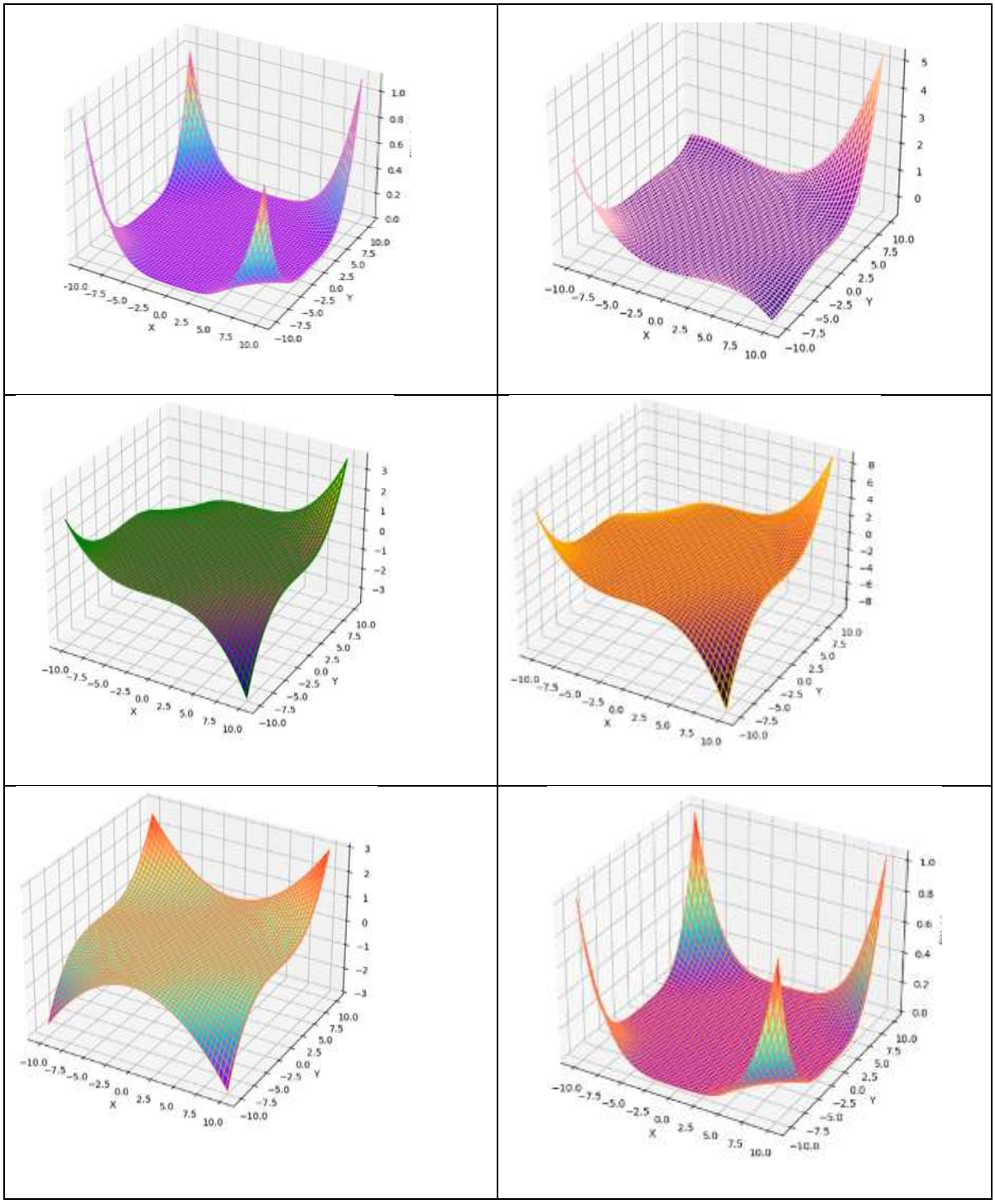
$$2(\mathrm{T}_a\mathrm{I})g(a,b) = \frac{178}{3}a^3 + \frac{141}{2}a^4 + \frac{244}{5}a^5 + 16a^6$$

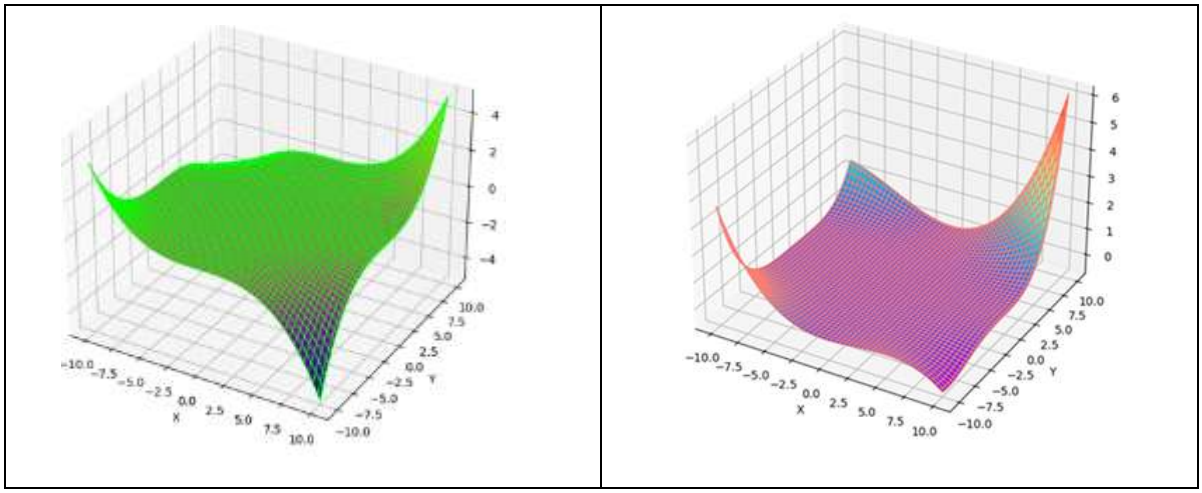
Presents the M-polynomials and $\bar{M}$ -polynomial graphical representations. First, we use a and b parameters to generate a horizontal grid, and then we build a surface on top of

that grid. Depending on the parameters, these graphs exhibit a variety of polynomial behaviour. We may control topological indices and co-indices. Consequently, a wide range of properties and activities by modifying the polynomials using these parameters.

7. Graph Analysis

Graphical representation of M-Polynomials&M̄- Polynomials for PolyketideAnitibiotics	
	
	
	





Conclusion:

In summary, this work has analyzed several topological properties of short-lived medications, including diorcinol, aspilactonol, ascomycotin, aspiketolactonol, aspyronol, engyodontiumone, and lindgomycin, through the application of various degree-based and vertex-based topological indices (Degree Based TIs and ValencyBased TIs). The findings highlight the significance of indices such as the F-index and reformulated Zagreb index (as effective molecular descriptors. These results serve as a basis for future studies aimed at employing these indices in the prediction of physicochemical properties via quantitative structure–activity, structure–property, and structure–toxicity relationships (QSAR, QSPR, QSTR). This research thereby contributes to enhancing the predictive capacity of topological indices in chemical and pharmaceutical analysis.

Author Contribution:

All Authors Contributed equally.

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Ethics declaration: Not applicable.

Data Availability:

No datasets were generated or analysed during the current study.

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