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FULL PAPER

Computing molecular descriptors of chitosan derivatives and its M-polynomial expressions

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The fundamental topology of the structure of chemical compounds can be better understood by the method of topological indices /numerical descriptors. Topological index depicts the chemical characteristic of a molecule in numerical form. Topological indices are used for modelling of physicochemical, biological, and pharmacokinetic properties of the compounds. It plays vital role in the QSAR/QSPR studies. Descriptor's ability to extract information typically depends on the type of molecular representation used and the specified algorithm. These numerical values help the researchers in choosing the right compound for the drug design. Chitin and chitosan derivatives act as excellent suppressor of anti-tumour and anticancer activities in living beings. The increasing morbidity and mortality rate worldwide is correlated with two most important diseases viz., obesity and diabetes. To improve health condition and prevention of chronic diseases such as asthma, arthritis, hepatitis, gastritis, atherosclerosis etc, chitin, chitosan and their derivatives play as immune-enhancing anti-inflammatory potential. As chitin and chitosan have remarkable applications discussed above, this work pinpoints on computing a polynomial from which topological indices can be extracted for specific values of the parameters. In this work, the focus is on a type of polynomial known as M-polynomial from which various 11 degree-based TIs are derived for molecular graph of chitosan derivatives such as α, β and γ -chitins.

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KEYWORDS

Topological indices; M-polynomial; chitosan derivatives; QSAR/QSPR studies.

Introduction

The natural biopolymers that can be processed easily in different forms are chitin and chitosan. They can be formed into membranes, sponges, micro-particles, scaffolds used in wound healing, drug delivery, gene therapy, and tissue engineering. Chitin is rigid, hard and white natural mucobiopolymer that is the second most copious biopolymer on the earth. Carbon, hydrogen, and oxygen combine to form compound such as saccharides also known as carbohydrates.

The smallest carbohydrates are the monosaccharides which in turn become polysaccharides by the formation of building blocks. A short chain of monosaccharides

refers to oligosaccharides, often produced by anabolic or catabolic process. Depending on the number of monosaccharides, it is classified as disaccharides having two monosaccharides, trisaccharide with three, tetra saccharides containing four, penta-saccharides having five and so on. Monosaccharides play a significant role in generating energy consumption. Their derivatives are found in important nucleic acids like DNA, ATP, RNA, and key components of coenzymes.

Carbohydrates in nonnumeric, oligomer, and polymeric form, plays crucial role in cell interactions, hormones, tumour metastasis, and antibody recognition. The deacetylation of chitin results in chitosan, which is non-toxic, biocompatible, and biodegradable [1, 2].

Chitin/chitosan show captivating physiological, biological, and pharmacological properties. Chitosan obtained from Porifera has multiple applications in the scaffolds of marine sponges. Because of its natural characteristics such as biocompatibility, biodegradability, non-toxicity, and humidity absorption, chitin and chitosan are suitable for various applications in many fields.

Biological activities and applications of chitin and chitosan derivatives

Various researchers vouch that chitin and chitosan are adaptable antimicrobials because of its intrinsic and extrinsic factors such as degree of polymerization, deacetylation, and effective dose in experimental methods. Chitosan imparts preferable antimicrobial activity than chitin due to its finer solubility property and free amine group. Most of the biological applications are possible due to the antimicrobial activity of chitin/chitosan and they are supported experimentally. The mechanism of antimicrobial suggested that the amino sugar may enter the cell and made complex with DNA by binding at low molecular weight constituents. It was also observed that DNA leads to the obstruction of transcription and translation process. To improve health condition and prevention of deep-rooted diseases like asthma, arthritis, hepatitis, gastritis, atherosclerosis etc., chitin, chitosan, and their derivatives play an immune-enhancing anti-inflammatory potential [3].

The study of these properties is witnessed by advocating them in animal models. The interactions of chitin/chitosan and their derivative products are reported to have significance in checking the bleeding by contracting tissues, platelet aggregation, and blood coagulation factors. The bleeding time is therapeutically proved to be brought to normal range in rabbit model when chitosan is used in the treatment.

One of the most common cardiovascular diseases is high blood pressure also known as hypertension. Based on the magnificent hemostatic activity, chitin and chitosan derivatives have been explored for over production of angiotensin II in which its enzyme plays a significant role. Supplementing chitosan normalizes the systolic blood pressure in human. The uncontrolled cell division because of environmental and physical factors leads to cancer. Chitin and chitosan derivatives act as excellent suppressor of anti-tumour and anticancer activities in living beings [4].

The increasing morbidity and mortality rate worldwide are correlated with two most important diseases such as obesity and diabetes.

Despite a lot of research in improving the diabetic medicine, there is a huge demand for the natural antidiabetic agents which cannot be considered as pharmaceutical agent. In this situation, chitin/chitosan derivatives show a reasonable antidiabetic and hypocholesteraemia activity directly or indirectly. Chitosan has been found effective against type 1 and type 2 diabetes. A natural cat-ionic polymer that is derived from chitin

is chitosan. It has received greater focus in drug delivery mainly because of its biodegradable, biocompatible, and non-toxic nature. The drug release is controlled because of the presence of amine groups and hydroxyl. Majority of the relevance of graph theory in chemistry facilitates the study of many tools such as topological indices, polynomials, distance-based indices, eigen values, and so on. These tools provide treasure of data regarding a chemical compound that correlates with its structure. A topological index is a numerical value which defines the topology of the structure of the molecule and helps in predicting a range of molecular properties. It has widened its applications in many fields such as pharmacological medicine, toxicity, and theoretical chemistry [5-8]. The models of QSPR/QSAR/QSTR of chemical compounds are used to design a drug as it depends on properties (physicochemical) with high degree of exactness [9-12].

Initially, Harold Wiener in 1947 introduced the first topological index, Wiener index which is distance-based index. Since then, numerous studies have resulted in the evaluation of various TIs by many researchers. The numerical invariant defines a relation between the physical structure and the chemical properties of the compounds.

Wiener affirmed that the Wiener index suits best with the boiling point of the alkane by modelling the index on QSPR, following which it was used to link the structure to their respective biological activities and to interpret various properties of the compounds [13, 14]. The most popular and the oldest index in QSAR and QSPR models is the Randic index [15, 16]. Subsequently, Bollobas and Erdos introduced the generalised version of Randic index [17]. An alternative of the Randic index was the Harmonic index, introduced by Fatlowicz.

The most accepted indices introduced in 1972 by Gutman and Trinajstic are the first and the second Zagreb indices [18].

They have been found very impressive in determining the total π -electron energy of molecules [19]. Ranjini *et al.* redefined the Zagreb indices for a graph G as redefined the first, the second, and the third Zagreb indices. The augmented Zagreb index is found to be best in estimating the heat of formation of alkanes [20]. The Forgotten index introduced by Gutman *et al.*, is found to be almost identical in prediction performance to that of the original Zagreb index. Forgotten index was further studied by Furtula [21]. Various physicochemical properties can be illustrated with a high degree of accuracy using neighbourhood degree sum-based TIs. Ghorbani *et al.* defined neighbourhood degree of vertices index named as third version of Zagreb index [22–23].

Later, it was learnt by Hosamani that there is a high association of neighbourhood-based indices with the entropy of octane isomers which resulted in the introduction of Sanskruti index [24]. There were several neighbourhood-based indices introduced by many researchers globally which are in use in the study of QSAR/QSPR/QSTR analysis [25-27].

M-polynomial

There are many tools in graph theory that play an important role in various fields. Polynomials are one such tool which contribute to the applications of graph theory [29-31]. There are many polynomials introduced, in which Hosoya polynomial [28] played a significant role in distance-based polynomials. Recently, degree-based polynomial was introduced in 2015 [32], known as M-polynomial and subsequently NM-polynomial [33] was introduced which is neighbourhood degree-based polynomial. This article focuses on computation of M-polynomial through which eleven degree-based topological indices are derived for chitosan and their derivatives.

These indices are helpful in the studies of theoretical chemistry, pharmaceutical research, drug design, and other fields. Because of its broad applications, M-polynomial is used to obtain the formulae for topological indices that are degree-based and play a key role to appreciate various properties of a molecular structure. It is always preferable to find a compressed way to obtain various TIs using a single polynomial. This results in the usage of M-polynomial [34, 35]. These polynomials help in the study and investigation of properties using topological indices (TIs). The prediction of characteristics of novel drugs depends on the features of a molecular compound through its molecular graph. Consider a molecular graph $G = (V, E)$, where $V(G)$ denotes vertex set and $E(G)$ denotes edge set. The common representations such as $u \in V(G)$ is a vertex and d(u) are the degree of the vertex u, denotes the number of edges incident to the vertex u [36-38].

Definition 1.

The M-polynomial for a graph G is defined as follow:

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

such that m_{ij}, where i, j ≥ 1 denotes the cardinality of edges uv ∈ E(G), where {d(u), d(v)}={i, j}. Here, d (u), d(v) indicates number of edges incident to the vertices u and v in G. The list of TIs derived from M-polynomial are presented in Table.

TABLE 1 The relationship between several topological indices with M-polynomial

Topological Index	Formula $\phi(d(u), d(v))$	Derivation from $f(x,y) = M(G; x, y)$
$M_1(G)$	$\sum_{uv \epsilon E(G)} [d(u) + d(v)]$	$(D_x + D_y)(f(x,y))_{x=1=y}$
$M_2(G)$	$\sum_{uv \epsilon E(G)} [d(u)\, d(v)]$	$(D_x D_y)(f(x,y))_{x=1=y}$
${}^{m}M_2(G)$	$\sum_{uv \epsilon E(G)} \left[\frac{1}{d(u)\, d(v)}\right]$	$(S_x S_y)(f(x,y))_{x=1=y}$
$ReZG_3(G)$	$\sum_{uv \epsilon E(G)} d(u)\, d(v)[d(u) + d(v)]$	$D_x D_y (D_x + D_y)(f(x,y))_{x=1=y}$
$F(G)$	$\sum_{uv \epsilon E(G)} [d^2(u) + d^2(v)]$	$(D_x^k + D_y^k)(f(x,y))_{x=1=y}$
$R_k(G)$	$\sum_{uv \epsilon E(G)} \{d(u)\, d(v)\}^k$	$(D_x^k D_y^k)(f(x,y))_{x=1=y}$
$RR_k(G)$	$\sum_{uv \epsilon E(G)} \frac{1}{\{d(u)\, d(v)\}^k}$	$(S_x^k S_y^k)(f(x,y))_{x=1=y}$
$SDD(G)$	$\sum_{uv \epsilon E(G)} \left[\frac{d^2(u) + d^2(v)}{d(u)\, d(v)}\right]$	$(D_x S_y + S_x D_y)(f(x,y))_{x=1=y}$
$H(G)$	$\sum_{uv \epsilon E(G)} \left[\frac{2}{d(u) + d(v)}\right]$	$2S_x J(f(x,y))_{x=1=y}$
$I(G)$	$\sum_{uv \epsilon E(G)} \left[\frac{d(u)\, d(v)}{d(u) + d(v)}\right]$	$S_x J D_x D_y (f(x,y))_{x=1=y}$

$$A(G) \qquad \sum_{uv\epsilon E(G)} \left\{\frac{d(u)\,d(v)}{d(u)+\,d(v)-2}\right\}^3 \qquad S_x^3 Q_{-2} J D_x^3 D_y^3 \big(\mathrm{f(x,y)}\big)_{\mathrm{x=1=y}}$$

Where,

$$D_x = \mathrm{x}\frac{\partial(f(\mathrm{x,y}))}{\partial \mathrm{x}}, \qquad D_y = \mathrm{y}\frac{\partial(f(\mathrm{x,y}))}{\partial \mathrm{y}}, \qquad S_x = \int_0^{\mathrm{x}} \frac{f(t,\mathrm{y})}{t}\,dt,$$

$$S_y = \int_0^{y} \frac{f(\mathrm{x},t)}{t}\,dt\,, \qquad J(\,f(x\,,y)) = f(\mathrm{x}\,,\mathrm{x}),\ \text{and} \qquad Q_k(\,f(\mathrm{x}\,,\mathrm{y})) = x^k f(\mathrm{x}\,,y).$$

Results and discussion

In this article, M-polynomial approach is employed to compute TIs for the derivatives of chitosan (Figure 1). Simple graphs are modelled for the molecular structure of chitosan derivatives viz., α, β, and γ-chitins. The tools used for computing these results comprise of vertex and edge partition along with combinatorial methods [39].

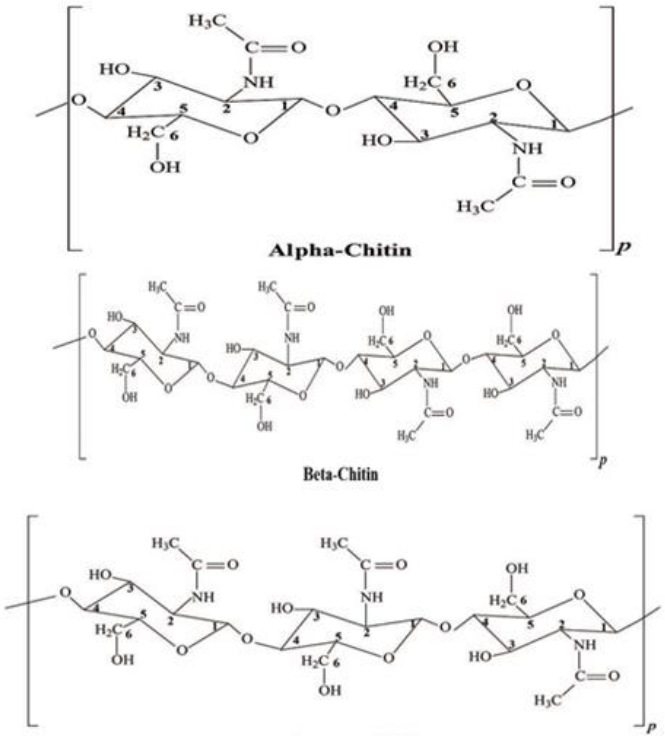

FIGURE 1 Structure of α, β, and γ-chitins

The significance of the study

Chitosan is the most abundant polysaccharide available after cellulose. It is a very useful compound that has found its applications in various fields because of its interesting properties. It plays a significant role in the drug delivery, food, textile, pharmacy, waste management, and diode. It has marvellous properties like healing, antimicrobial, and antifungal which are significant in drug making. Hydro gels formed by chitosan have attracted lots of attention in the pharmaceutical field in the usage of lysozyme and fabrication of dressings.

It will suck wound secretions and govern the hydration of the wounded region. Chitosan derivatives are proven to be the safest choice in the applications of biomaterials that are extensively used for medical purposes. It is evident that there is a large volume of studies taking place on

polysaccharide [40, 41] gradable, polymer membranes, and nano-fibres in the medical field. A class of materials that are integrated from chitosan and its derivatives are hydrogels used in producing contact lenses, wound dressings, and hygiene products. The significant characteristics and natural abundance of chitosan (hydrogels) like malleability, non-toxicity, and biocompatibility have attracted lot of studies from academia and industry [42].

M-polynomial of α-chitin

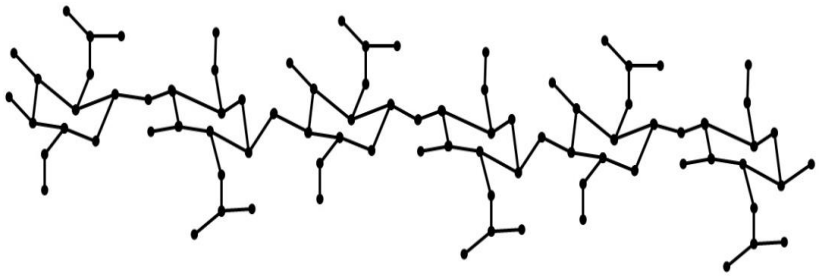

FIGURE 2 α -chitin molecular graph with p=3

Theorem 1

The M-polynomial for α-chitin is

$M(\alpha C; x, y) = (2p)xy^2 + (6p + 2)xy^3 + (14p - 2)x^2y^3 + (8p)x^3y^3$.

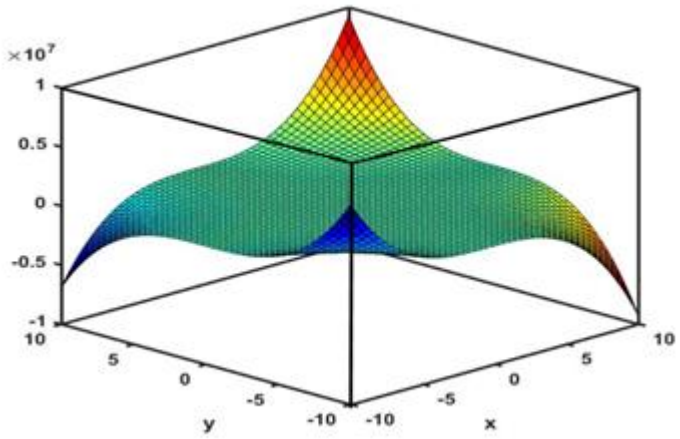

FIGURE 3 M-polynomial of α-chitin 3D plot

Proof

Based on the Figure 2, it is observed that $|V(\alpha C)| = 28p + 1$ and $|E(\alpha C)| = 30p$. Also, the edge set of αC is classified into four edge partitions depending on the vertex degrees are given as follow:

$E_{12} = \{uv \in E(\alpha C)/d(u) = 1, d(v) = 2\}$,
$E_{13} = \{uv \in E(\alpha C)/d(u) = 1, d(v) = 3\}$,
$E_{23} = \{uv \in E(\alpha C)/d(u) = 2, d(v) = 3\}$,
$E_{33} = \{uv \in E(\alpha C)/d(u) = 3, d(v) = 3\}$,

such that

$m_{12} = 2p$, $m_{13} = 6p + 2$, $m_{23} = 14p - 2$, and $m_{33} = 8p$.

Using the definition 1,

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

$$M(\alpha C; x, y) = \sum_{1\le 2} m_{12}\, x^1 y^2 + \sum_{1\le 3} m_{13}\, x^1 y^3 + \sum_{2\le 3} m_{23}\, x^2 y^3 + \sum_{3\le 3} m_{33}\, x^3 y^3$$

$= (2p)xy^2 + (6p + 2)xy^3 + (14p - 2)x^2y^3 + (8p)x^3y^3$.

TIs of α-chitin are computed using Theorem 1 and Table 1, and is as follow:

Proposition 1

$M_1(\alpha C) = 148p - 2$.
$M_2(\alpha C) = 178p - 6$.
${}^mM_2(\alpha C) = 6.222p + 0.333$.
$ReZG_3(\alpha C) = 936p - 36$.
$F(\alpha C) = 396p - 6$
$R_k(\alpha C) = 2^k(2p) + 3^k(6p + 2) + 6^k(14p - 2) + 3^{2k}(8p)$.
$RR_k(\alpha C) = \frac{(2p)}{2^k} + \frac{(6p+2)}{3^k} + \frac{(14p-2)}{6^k} + \frac{(8p)}{3^{2k}}$.
$SDD(\alpha C) = 71.332p + 2.333$.
$H(\alpha C) = 12.6p + 0.2$.
$I(\alpha C) = 34.633p - 0.9$.
$A(\alpha C) = 239.375p - 9.25$.

Proof

Let $f(x, y) = M(\alpha C; x, y) = (2p)xy^2 + (6p + 2)xy^3 + (14p - 2)x^2y^3 + (8p)x^3y^3$.
Then,
$D_x f(x, y) = (2p)x^1y^2 + (6p + 2)x^1y^3 + 2(14p - 2)x^2y^3 + 3(8p)x^3y^3$,
$D_y f(x, y) = 2(2p)\, x^1y^2 + 3(6p + 2)\, x^1y^3 + 3(14p - 2)\, x^2y^3 + 3(8p)\, x^3y^3$,
$(D_x + D_y) f(x, y) = 3(2p)\, x^1y^2 + 4(6p + 2)\, x^1y^3 + 5(14p - 2)\, x^2y^3 + 6(8p)\, x^3y^3$,
$D_yD_xf(x, y) = 2(2p)\, x^1y^2 + 3(6p + 2)\, x^1y^3 + 6(14p - 2)\, x^2y^3 + 9(8p)\, x^3y^3$,
$(D^2_x + D^2_y) f(x, y) = 5(2p)\, x^1y^2 + 10(6p + 2)\, x^1y^3 + 13(14p - 2)\, x^2y^3 + 18(8p)\, x^3y^3$,
$D^k_xD^k_yf(x, y) = 2^k(2p)\, x^1y^2 + 3^k(6p + 2)\, x^1y^3 + 6^k(14p - 2)\, x^2y^3 + 3^{2k}(8p)\, x^3y^3$,
$D_x D_y (D_x + D_y) f(x, y) = 6(2p)\, x^1y^2 + 12(6p + 2)\, x^1y^3 + 30(14p - 2)\, x^2y^3 + 54(8p)\, x^3y^3$,
$S_xS_y f(x, y) = \frac{(2p)}{2}xy^2 + \frac{(6p+2)}{3}xy^3 + \frac{(14p-2)}{6}x^2y^3 + \frac{(8p)}{9}x^3y^3$,
$S^k_xS^k_yf(x, y) = \frac{(2p)}{2^k}xy^2 + \frac{(6p+2)}{3^k}xy^3 + \frac{(14p-2)}{6^k}x^2y^3 + \frac{(8p)}{3^{2k}}x^3y^3$.
$(S_yD_x + S_xD_y)f(x, y) = \frac{5(2p)}{2}xy^2 + \frac{10(6p+2)}{3}xy^3 + \frac{13(14p-2)}{6}x^2y^3 + \frac{18(8p)}{9}x^3y^3$,
$S_x Jf(x, y) = \frac{(2p)}{3}x^3 + \frac{(6p+2)}{4}x^4 + \frac{(14p-2)}{5}x^5 + \frac{(8p)}{6}x^6$,
$S_x JD_x D_y f(x, y) = \frac{2(2p)}{3}x^3 + \frac{3(6p+2)}{4}x^4 + \frac{6(14p-2)}{5}x^5 + \frac{9(8p)}{6}x^6$,
$S^3_xQ_{-2}JD^3_xD^3_y f(x, y) = \frac{(2)^3(2p)}{(1)^3}x^1 + \frac{(3)^3(6p+2)}{(2)^3}x^2 + \frac{(6)^3(14p-2)}{(3)^3}x^3 + \frac{(9)^3(8p)}{(4)^3}x^4$,

According to Table 1, the following results are obtained:
$M_1(\alpha C) = (D_x + D_y)f(x, y)\,|_{x=1=y} = 148p - 2$.
$M_2(\alpha C) = (D_xD_y)\, f(x, y)|_{x=1=y} = 178p - 6$.
${}^mM_2(\alpha C) = (S_xS_y)f\,(x, y)|_{x=1=y} = 6.222p + 0.333$.
$ReZG_3(\alpha C) = D_xD_y(D_x + D_y)\, f(x, y)|_{x=1=y} = 936p - 36$.
$F(\alpha C) = (D^2_x + D^2_y)\, f(x, y)|_{x=1=y} = 396p - 6$.
$R_k(\alpha C) = (D^k_xD^k_y)\, f(x, y)|_{x=1=y} = 2^k\,(2p) + 3^k\,(6p + 2) + 6^k\,(14p - 2) + 3^{2k}\,(8p)$.
$RR_k(\alpha C) = (S^k_xS^k_y)\, f(x, y)|_{x=1=y} = \frac{(2p)}{2^k} + \frac{(6p+2)}{3^k} + \frac{(14p-2)}{6^k} + \frac{(8p)}{3^{2k}}$.
$SDD(\alpha C) = (S_yD_x + S_xD_y)\, f(x, y)|_{x=1=y} = 71.332p + 2.333$.
$H(\alpha C) = 2S_x J\, f(x, y)|_{x=1=y} = 12.6p + 0.2$.
$I(\alpha C) = S_x J\, D_x D_y f(x, y)|_{x=1=y} = 34.633p - 0.9$.
$A(\alpha C) = S^3_xQ_{-2}\, J\, D^3_x\, D^3_y f(x, y)|_{x=1=y} = 239.375p - 9.25$.

M-polynomial of β-chitin (βC)

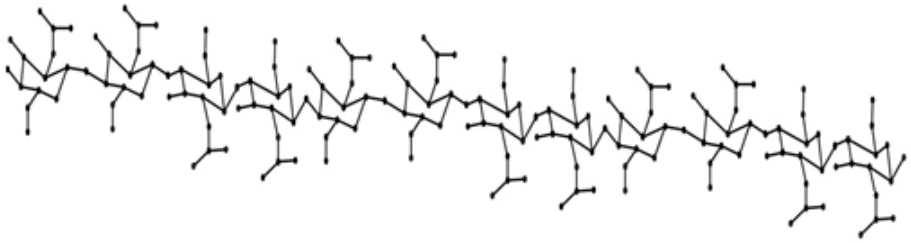

FIGURE 4 β-chitin molecular graph with p=3

Theorem 2

The M-polynomial for β-chitin is as follow:

$M(\beta C; x, y) = (4p)xy^2 + (12p + 2)xy^3 + (28p - 2)x^2y^3 + (16p)x^3y^3$.

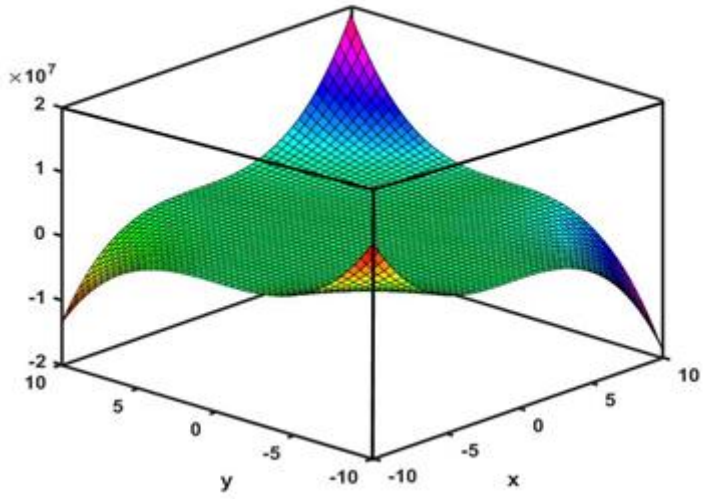

FIGURE 5 M-polynomial of β-chitin in 3D plot

Proof

The vertex and edge partitions of beta chitin from the Figure 4 are found to be $|V(\beta C)| = 55p + 2$ and $|E(\beta C)| = 60p$, respectively. The edge set of βC based on vertex degrees are given by

$E_{12} = \{uv \in E(\beta C) | d(u) = 1, d(v) = 2\}$,
$E_{13} = \{uv \in E(\beta C) | d(u) = 1, d(v) = 3\}$,
$E_{23} = \{uv \in E(\beta C) | d(u) = 2, d(v) = 3\}$,
$E_{33} = \{uv \in E(\beta C) | d(u) = 3, d(v) = 3\}$,

such that

$m_{12} = 4p$, $m_{13} = 12p + 2$, $m_{23} = 28p - 2$, and $m_{33} = 16p$.

Using definition 1,

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

$$M(\beta C; x, y) = \sum_{1 \le 2} m_{12} x^1 y^2 + \sum_{1 \le 3} m_{13} x^1 y^3 + \sum_{2 \le 3} m_{23} x^2 y^3 + \sum_{3 \le 3} m_{33} x^3 y^3$$

$= (4p)xy^2 + (12p + 2)xy^3 + (28p - 2)x^2y^3 + (16p)x^3y^3$.

From Theorem 2 and Table 1, various degree-based TIs of β-chitin are given by Proposition 2.

$M_1(\beta C) = 296p - 2.$
$M_2(\beta C) = 356p - 6.$
$^mM_2(\beta C) = 12.444p + 0.333.$
$ReZG_3(\beta C) = 1872p - 36.$
$F(\beta C) = 792p - 6.$
$R_k(\beta C) = 2^k(4p) + 3^k(12p + 2) + 6^k(28p - 2) + 32^k(16p).$
$RR_k(\beta C) = \frac{(4p)}{2^k} + \frac{(12p+2)}{3^k} + \frac{(28p-2)}{6^k} + \frac{(16p)}{3^{2k}}.$
$SDD(\beta C) = 142.666p + 2.333.$
$H(\beta C) = 25.199p + 0.2.$
$I(\beta C) = 69.266p - 0.9.$
$A(\beta C) = 478.75p - 9.25.$

Proof

Let $f(x, y) = M(\beta C; x, y) = (4p)xy^2 + (12p + 2)xy^3 + (28p - 2)x^2y^3 + (16p)x^3y^3.$

Then,

$D_xf(x, y) = (4p)x^1y^2 + (12p + 2)x^1y^3 + 2(28p - 2)x^2y^3 + 3(16p)x^3y^3,$
$D_yf(x, y) = 2(4p)x^1y^2 + 3(12p+2)x^1y^3 + 3(28p - 2)x^2y^3 + 3(16p)x^3y^3,$
$(D_x + D_y)f(x, y) = 3(4p)x^1y^2 + 4(12p + 2)x^1y^3 + 5(28p - 2)x^2y^3 + 6(16p)x^3y^3,$
$D_yD_xf(x, y) = 2(4p)x^1y^2 + 3(12p + 2)x^1y^3 + 6(28p - 2)x^2y^3 + 9(16p)x^3y^3,$
$(D^2_x + D^2_y)f(x, y) = 5(4p)x^1y^2 + 10(12p + 2)x^1y^3 + 13(28p - 2)x^2y^3 + 18(16p)x^3y^3,$
$D^k_xD^k_yf(x, y) = 2^k(4p)x^1y^2 + 3^k(12p + 2)x^1y^3 + 6^k(28p - 2)x^2y^3 + 3^{2k}(16p)x^3y^3,$
$D_xD_y(D_x+D_y)f(x, y) = 6(4p)x^1y^2 + 12(12p + 2)x^1y^3 + 30(28p - 2)x^2y^3 + 54(16p)x^3y^3,$
$S_xS_yf(x, y) = \frac{(4p)}{2}xy^2 + \frac{(12p+2)}{3}xy^3 + \frac{(28p-2)}{6}x^2y^3 + \frac{(16p)}{9}x^3y^3,$
$S^k_xS^k_yf(x, y) = \frac{(4p)}{2^k}xy^2 + \frac{(12p+2)}{3^k}xy^3 + \frac{(28p-2)}{6^k}x^2y^3 + \frac{(16p)}{3^{2k}}x^3y^3,$
$(S_yD_x + S_xD_y)f(x, y) = \frac{5(4p)}{2}xy^2 + \frac{10(12p+2)}{3}xy^3 + \frac{13(28p-2)}{6}x^2y^3 + \frac{18(16p)}{9}x^3y^3,$
$S_xJf(x, y) = \frac{(4p)}{3}x^3 + \frac{(12p+2)}{4}x^4 + \frac{(28p-2)}{5}x^5 + \frac{(16p)}{6}x^6,$
$S_xJD_xD_yf(x, y) = \frac{2(4p)}{3}x^3 + \frac{3(12p+2)}{4}x^4 + \frac{6(28p-2)}{5}x^5 + \frac{9(16p)}{6}x^6,$
$S^3_xQ_{-2}JD^3_xD^3_y f(x, y) = \frac{(2)^3(4p)}{(1)^3}x^1 + \frac{(3)^3(12p+2)}{(2)^3}x^2 + \frac{(6)^3(28p-2)}{(3)^3}x^3 + \frac{(9)^3(16p)}{(4)^3}x^4,$

Using Table 1, the following results are obtained as follow:

$M_1(\beta C) = (D_x + D_y)f(x, y)|_{x=1=y} = 296p - 2.$
$M_2(\beta C) = (D_xD_y)f(x, y)|_{x=1=y} = 356p - 6.$
$^mM_2(\beta C) = (S_xS_y)f(x, y)|_{x=1=y} = 12.444p + 0.333.$
$ReZG_3(\beta C) = (D_xD_y)(D_x + D_y)f(x, y)|_{x=1=y} = 31872p - 36.$
$F(\beta C) = (D^2_x + D^2_y)f(x, y)|_{x=1=y} = 792p - 6.$
$R_k(\beta C) = (D^k_xD^k_y)f(x, y)|_{x=1=y} = 2^k(4p) + 3^k(12p + 2) + 6^k(28p - 2) + 3^{2k}(16p).$
$RR_k(\beta C) = (S^k_xS^k_y)f(x, y)|_{x=1=y} = (4p)2^k + (12p + 2)3^k + (28p - 2)6^k + (16p)3^{2k}.$
$SDD(\beta C) = (D_xS_y + S_xD_y)f(x, y)|_{x=1=y} = 142.666p + 2.333.$
$H(\beta C) = 2S_xJf(x, y)|_{x=y=1} = 25.199p + 0.2.$

$I(\beta C) = S_xJD_xD_yf(x, y)|_{x=y=1} = 69.266p - 0.9.$

$A(\beta C) = S^3_xQ_{-2}JD^3_xD^3_y f(x, y)|_{x=y=1} = 478.75p - 9.$

M-polynomial of γ-chitin(γC)

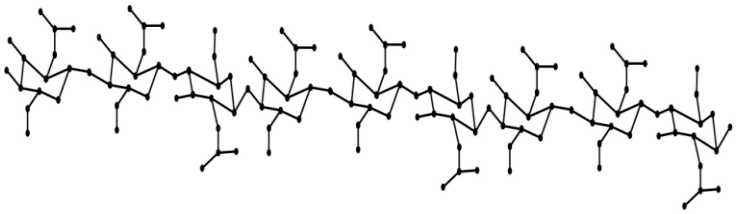

FIGURE 6 γ-chitin molecular graph with $p = 3$

Theorem 3

The M-polynomial for γ-chitin is:

$M(\gamma C; x, y) = (3p)xy^2 + (9p + 2)xy^3 + (21p - 2)x^2y^3 + (12p)x^3y^3$.

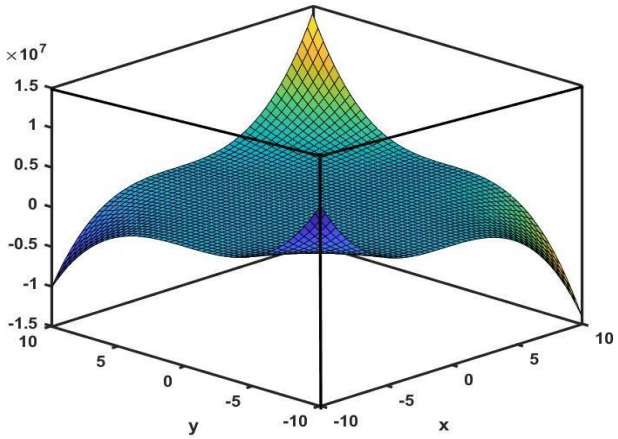

FIGURE 7 M-polynomial of γ-chitin in 3D plot

Proof

Based the Figure 6, it is observed that |V (γC)| = 28p+1 and |E(γC)| = 30p. Also, the edge set of γC is classified into four edge partitions depending on the vertex degrees are given as follow:

$E_{12} = \{uv \in E(\gamma C) | d(u) = 1, d(v) = 2\}$,
$E_{13} = \{uv \in E(\gamma C) | d(u) = 1, d(v) = 3\}$,
$E_{23} = \{uv \in E(\gamma C) | d(u) = 2, d(v) = 3\}$,
$E_{33} = \{uv \in E(\gamma C) | d(u) = 3, d(v) = 3\}$,
such that
$m_{12} = 3p$, $m_{13} = 9p + 2$, $m_{23} = 21p - 2$, and $m_{33} = 12p$.

Using definition 1,

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

$$M(\gamma C; x, y) = \sum_{1 \le 2} m_{12} x^1 y^2 + \sum_{1 \le 3} m_{13} x^1 y^3 + \sum_{2 \le 3} m_{23} x^2 y^3 + \sum_{3 \le 3} m_{33} x^3 y^3$$

$= (3p)xy^2 + (9p + 2)xy^3 + (21p - 2)x^2y^3 + (12p)x^3y^3$.

Using Theorem 3 and Table 1, various degree-based TIs of the γ-chitin are given as follow:

Proposition 3

$M_1(\gamma C) = 222p - 2$.
$M_2(\gamma C) = 267p - 6$.
${}^mM_2(\gamma C) = 9.333p + 0.333$.
$ReZG_3(\gamma C) = 1404p - 36$.
$F(\gamma C) = 594p - 6$.
$R_k(\gamma C) = 2^k(3p) + 3^k(9p + 2) + 6^k(21p - 2) + 3^{2k}(12p)$.
$RR_k(\gamma C) = \frac{(3p)}{2^k} + \frac{(9p + 2)}{3^k} + \frac{(21p - 2)}{6^k} + \frac{(12p)}{3^{2k}}$.
$SDD(\gamma C) = 106.998p + 2.333$.
$H(\gamma C) = 18.899p + 0.2$.
$I(\gamma C) = 51.95p - 0.9$.
$A(\gamma C) = 359.062p - 9.25$.

Proof

Let $f(x, y) = (3p)xy^2 + (9p + 2)xy^3 + (21p - 2)x^2y^3 + (12p)x^3y^3$.

Then,

$D_x f(x, y) = (3p)x^1y^2 + (9p + 2)x^1y^3 + 2(21p - 2)x^2y^3 + 3(12p)x^3y^3$,
$D_y f(x, y) = 2(3p)x^1y^2 + 3(9p + 2)x^1y^3 + 3(21p - 2)x^2y^3 + 3(12p)x^3y^3$,
$(D_x + D_y) f(x, y) = 3(3p)x^1y^2 + 4(9p + 2)x^1y^3 + 5(21p - 2)x^2y^3 + 6(12p)x^3y^3$,

$D_y\ D_x\ f(x, y) = 2(3p)\ x^1y^2 + 3(9p + 2)x^1y^3 + 6(21p - 2)\ x^2y^3 + 9(12p)\ x^3y^3$,

$(D^2_x + D^2_y)f(x, y) = 5(3p)\ x^1y^2 + 10(9p + 2)x^1y^3 + 13(21p - 2)\ x^2y^3 + 18(12p)\ x^3y^3$,

$D^k_x\ D^k_y\ f(x, y) = 2^k\ (3p)\ x^1y^2 + 3^k\ (9p + 2)\ x^1y^3 + 6^k\ (21p - 2)\ x^2y^3 + 3^{2k}\ (16p)\ x^3y^3$,

$D_x\ D_y(D_x+D_y)f(x, y) = 6(3p)\ x^1y^2 + 12(9p + 2)x^1y^3 + 30(21p - 2)\ x^2y^3 + 54(12p)\ x^3y^3$,

$S_x\ S_yf(x, y) = \frac{(3p)}{2}xy^2 + \frac{(9p + 2)}{3}xy^3 + \frac{(21p - 2)}{6}x^2y^3 + \frac{(12p)}{9}\ x^3y^3$,

$S^k_x\ S^k_yf(x, y) = \frac{(3p)}{2^k}\ xy^2 + \frac{(9p + 2)}{3^k}\ xy^3 + \frac{(21p - 2)}{6^k}x^2y^3 + \frac{(12p)}{3^{2k}}\ x^3y^3$.

$(S_yD_x + S_xD_y)f(x, y) = \frac{5(3p)}{2}xy^2 + \frac{10\ (9p + 2)}{3}xy^3 + \frac{13(21p - 2)}{6}x^2y^3 + \frac{18(12p)}{9}\ x^3y^3$,

$S_x J\ f(x, y) = \frac{(3p)}{3}x^3 + \frac{(9p + 2)}{4}x^4 + \frac{(21p - 2)}{5}x^5 + \frac{(12p)}{6}\ x^6$,

$S_x\ J\ D_x\ D_yf(x, y) = \frac{2(3p)}{3}x^3 + \frac{3(9p + 2)}{4}x^4 + \frac{6(21p - 2)}{5}x^5 + 9\frac{(12p)}{6}\ x^6$,

$S^3_xQ_{-2}JD^3_xD^3_y\ f(x, y) = \frac{(2)^3\ (3p)}{(1)^3}x^1 + \frac{(3)^3(9p + 2)}{(2)^3}x^2 + \frac{(6)^3(21p - 2)}{(3)^3}x^3 + \frac{(9)^3(12p)}{(4)^3}\ x^4$,

Using Table 1, we obtain the following results:

$M_1(\gamma C) = (D_x + D_y)f(x, y)|_{x=1=y} = 222p - 2.$

$M_2(\gamma C) = (D_x\ D_y)f(x, y)|_{x=1=y} = 267p - 6.$

$^mM_2(\gamma C) = S_xS_yf(x, y)|_{x=1=y} = 9.333p + 0.333.$

$ReZG_3(\gamma C) = (D_x\ D_y)\ (D_x + D_y)f(x, y)|_{x=1=y} = 1404p - 36.$

$F(\gamma C) = (D^2_x + D^2_y)f(x, y)|_{x=1=y} = 594p - 6.$

$R_k(\gamma C) = (D^k_xD^k_y)f(x, y)|_{x=1=y} = 2^k\ (3p) + 3^k\ (9p + 2) + 6^k\ (21p - 2) + 32^k\ (12p).$

$RR_k(\gamma C) =) = \frac{(3p)}{2^k} + \frac{(9p + 2)}{3^k} + \frac{(21p - 2)}{6^k} + \frac{(12p)}{3^{2k}}$.

$(S^k_xS^k_y)f(x, y)|_{x=1=y} = \frac{(3p)}{2^k} + \frac{(9p + 2)}{3^k} + \frac{(21p - 2)}{6^k} + \frac{(12p)}{3^{2k}}$.

$SDD(\gamma C) = (D_xS_y + S_xD_y)f(x, y)|_{x=1=y} = 106.998p + 2.333.$

$H(\gamma C) = 2S_xJf(x, y)|_{x=y=1} = 18.899p + 0.2.$

$I(\gamma C) = S_xJD_xD_yf(x, y)|_{x=y=1} = 51.95p - 0.9.$

$A(\gamma C) = S^3_xQ_{-2}JD^3_xD^3_y\ f(x, y)|_{x=y=1} = 359.062p - 9.25$

Comparison of indices using numerical data

Eleven topological indices are derived and computed for the chitosan derivatives and a detailed comparison is tabulated through Tables 2 to 4 for different values of n = 1 to 10. The TIs follow an upward trend as n increases.

TABLE 2 Comparison of degree-based TIs of α-chitin for n = 1 to 10 using numerical data

n	M_1	M_2	$^mM_2$	$ReZG_3$	F	R	RR	SDD	H	I	A
1	146	172	6.555	900	390	13.597	70.078	73.665	12.8	33.733	230.125
2	294	350	12.777	1836	786	26.856	141.591	144.997	25.4	68.366	469.5
3	442	528	8.999	2772	1182	40.115	213.104	216.329	38	108.999	708.875
4	590	706	25.221	3708	1578	53.374	284.617	287.661	50.6	137.632	948.25
5	738	884	31.443	4644	1974	66.633	356.13	358.993	63.2	172.265	1187.6
6	886	1062	37.665	5580	2370	79.892	427.643	430.325	75.8	206.898	1427

7	1034	1240	43.887	6516	2766	93.151	499.156	501.657	88.4	241.531	1666.4
8	1182	1418	50.109	7452	3162	106.41	570.669	572.989	101	276.164	1905.8
9	1330	1596	56.331	8388	3558	119.669	642.182	644.321	113.6	310.797	2145.1
10	1478	1774	62.553	9324	3954	132.928	713.695	715.653	126.2	345.43	2384.5

TABLE 3 Comparison of degree-based TIs of β-chitin for n = 1 to 10 using numerical data

n	M_1	M_2	$^mM_2$	$ReZG_3$	F	R	RR	SDD	H	I	A
1	294	350	12.777	1836	786	26.856	141.592	145.003	25.399	68.367	469.5
2	590	706	25.221	3708	1578	53.375	284.619	287.673	50.598	137.634	948.25
3	886	1062	37.665	5580	2370	79.893	427.646	430.343	75.7976	206.901	1427
4	1182	1418	50.109	7452	3162	106.412	570.673	573.013	100.997	276.168	1905.8
5	1478	1774	62.553	9324	3954	132.930	713.7	715.683	126.196	345.435	2384.5
6	1774	2130	74.997	11196	4746	159.449	856.727	858.353	151.395	414.702	2863.3
7	2070	2486	87.441	13068	5538	185.967	999.754	1001	176.594	483.969	3342
8	2366	2842	99.885	14940	6330	212.485	1142.8	1143.7	201.794	553.236	3820.8
9	2662	3198	112.329	16812	7122	239.004	1285.8	1286.4	226.993	622.503	4299.5
10	2958	3554	124.773	18684	7914	265.522	1428.8	1429	252.192	691.77	4778.3

TABLE 4 Comparison of degree-based indices of γ-chitin for n = 1 to 10 using numerical data

n	M_1	M_2	$^mM_2$	$ReZG_3$	F	R	RR	SDD	H	I	A
1	220	261	9.666	1368	588	20.228	105.835	109.332	19.099	51.05	349.812
2	442	528	18.999	2772	1182	40.118	213.105	216.33	37.998	102.999	708.874
3	664	795	28.333	4176	1776	60.008	320.375	323.328	56.898	154.949	1067.9
4	886	1062	37.666	5580	2370	79.898	427.645	430.327	75.798	206.899	1427

5	1108	1329	46.999	6984	2964	99.788	534.915	537.325	94.697	258.849	1786.1
6	1330	1596	56.333	8388	3558	119.678	642.185	644.323	113.596	310.799	2145.1
7	1552	1863	65.666	9792	4152	139.568	749.455	751.321	132.496	362.749	2504.2
8	1774	2130	74.999	11196	4746	159.458	856.725	858.319	151.395	414.698	2863.2
9	1996	2397	84.333	12600	5340	179.348	963.995	965.318	170.294	466.648	3222.3
10	2218	2664	96.666	14004	5934	199.238	1071.3	1072.3	189.194	518.598	3581.4

Conclusion

A biodegradable polymer that is obtained from chitin is chitosan. It has varied applications in biomedical, textile, food storage, and many other fields. Hydrogels formed by chitosan are extensively used in medicines as they are absorbents of water-based liquids in the wounded areas. Chitosan is used as antimicrobial textiles for wound dressings. They are often used in drugs and proteins due to their inherent characteristics like non-toxicity, biocompatibility, hydrophilicity, etc. Chitosan finds its applications in technology as adsorbent of metals and dyes in waste-water from industrials wastes. This article focusses on finding M-polynomial of chitosan derivatives from which eleven degree-based TIs are computed. Thorough comparisons of the indices are tabulated. These polynomials are graphically represented in 3D plots (Figures 3, 5, and 7). The compounds used in drug discovery will be edible based on the range of topological indices. If the value of the index does not come under that range, it cannot be used as an excipient as it has to be consumed by the living beings. The compounds under this study include ample applications, and hence this study would be useful appropriately for the researchers who are willing to work on the same compounds.

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Authors' contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

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