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Research Article

M-Polynomial and NM-Polynomial Methods for Topological Indices of Polymers

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Topological indices (TIs) are numerical tools widely applied in chemometrics, biomedicine, and bioinformatics for predicting diverse physicochemical attributes and biological activities within molecular structures. Despite their significance, the challenges in deriving TIs necessitate novel approaches. This study addresses the limitations of conventional methods in dealing with dynamic molecular structures, focusing on the neighborhood M-polynomial (NM-polynomial), a pivotal polynomial for calculating degree-based TIs. Current literature acknowledges these polynomials but overlooks their limited adaptability to intricate biopolymer relationships. Our research advances by computing degree-based and neighborhood degree-based indices for prominent biopolymers, including polysaccharides, poly-γ-glutamic acid, and poly-L-lysine. Through innovative utilization of the NM-polynomial and the M-polynomial, we establish a fresh perspective on molecular structure and topological indices. Moreover, we present diverse graph representations highlighting the nuanced correlations between indices and structural parameters. By systematically investigating these indices and their underlying polynomials, our work contributes to predictive modelling in various fields. This exploration sheds light on intricate biochemical systems, offering insights into applications encompassing medicine, the food industry, and wastewater treatment. This research deepens our understanding of complex molecular interactions and paves the way for enhanced applications in diverse industries.

1. Introduction

Graph theory finds application in various fields, with one prominent branch being chemical graph theory (CGT). CGT is utilized to study chemical compounds and predict their distinctive properties. The concept of a molecular graph employs the arrangement and connections of components in a molecule to forecast its boiling point. This association is valuable for creating chemical processes, synthetic materials, and chemical assembly lines. Chemists employ diverse physical attributes to fathom molecular structures. Topological indices (TIs) predict physicochemical traits and biological activities of bioactive compounds, while also holding promise for predicting substance hazards. TIs offer an avenue to forecast drug behavior based on their electronic structures, offering an alternative to empirical testing. TIs have been instrumental in characterizing the physical properties of alkenes and projecting boiling points for untested alkanes. See [1–3] for insights into alkenes' physical properties.

Since 1947, topological indices (TIs) have evolved, categorized by distinct graph attributes such as vertex degrees, intervertex distances, and graph eigenvalues, and using characteristic graph notation. However, some TIs are not directly calculable, prompting the development of polynomials as a solution. The degree-dependent M-polynomial, assessing degree-based TIs, is one such polynomial. The neighborhood M-polynomial, linked to the sum of neighborhood vertex degrees, is another alternative. These indices' closed equations for a graph family are deduced by computing the graph family's M-polynomial and NM-polynomial.

The M-polynomial aggregates pertinent degree-based TIs into a polynomial framework. E. Deutsch and S. Klavár introduced the M-polynomial in 2015, gaining wide acceptance. In 2018, Mondal et al. extended this with the neighborhood M-polynomial, focusing on degree-centered neighborhood indices. The NM-polynomial has facilitated the generation of neighborhood degree-based TIs for structures such as cuprous oxide's crystalline form and the face-centered cubic lattice. Subsequent studies, including those by Havare [4] and Mondal et al. [5, 6], have further advanced this field.

Polysaccharide-based drug delivery vehicles represent a promising avenue due to biodegradability, low immunogenicity, and improved pharmacokinetics. These vehicles, incorporating drug-loaded polysaccharides, offer controlled and safer delivery with fewer adverse effects compared to conventional vectors. Polysaccharides ensure sustained drug release, boasting superior safety and high physiological tolerance. Notably, polysaccharides have facilitated novel drug distribution mechanisms, as seen in "Novochizol" for COVID-19 treatment [7].

Gamma-PGAs are gaining traction in drug delivery for their nontoxicity, water solubility, biodegradability, and biocompatibility. Gamma-PGA's monomer units sport free carboxyl groups, enabling coupling with other polymers or active compounds and self-assembly into amphiphilic nanoparticles with hydrophobic esters. This system is particularly beneficial for poorly water-soluble drugs. Gamma-PGA has broad applications, including cancer therapy, gene therapy, biological adhesives, and vaccines [8].

Poly-L-lysine (PLL), a highly positively charged amino acid chain, enhances cell adhesion and growth in culture. Coating cultureware with PLL boosts cell adhesion, relying on the attraction between positively and negatively charged molecules or cells. Poly-D-lysine (PDL) and PLL enhance cell attachment to surfaces and offer resistance to enzymatic degradation, thus prolonging adherence [9]. PLL's positive charge density enables binding to negatively charged macromolecules, forming soluble complexes. This attribute is leveraged for DNA and protein delivery [10, 11]. Polylysine-based nanoparticles passively accumulate at sites of vascular damage, offering a novel method for targeted treatment [12].

The study's core objective is to evaluate topological indices (TIs) for polysaccharide, poly-γ-glutamic acid, and poly-l-lysine, utilizing M-polynomial and NM-polynomial calculations. These indices are computed through the edge partition method and combinatorial analysis, aiding research into medication structure's physicochemical traits. Various TIs fall into categories such as degree-based [13, 14], distance-based [15–17], spectrum-based [15, 18, 19], or status-based [18, 20] indices, with recent research exploring TIs' predictive potential for diverse physicochemical properties.

2. M-Polynomial and NM-Polynomial

Polynomials, a key graph theory tool, find wide applications [21–25]. The Hosoya polynomial [26] is pivotal for distance-oriented topological indices. The M-polynomial, introduced by Deutsch and Klav zar in 2015 [27], is a foundational tool, as is the NM-polynomial by Mondal et al. in 2018 [28], for closed-form degree-based topological indices. The M-polynomial generates many crucial indices, adapting swiftly to new index creation. Recent emphasis on neighborhood degree sum-based indices has fueled research into NM-polynomials. The M-polynomial corresponds to degree-constructed indices, while the NM-polynomial parallels this for neighborhood degree-based indices.

The M-polynomial and NM-polynomial's calculation for biopolymer structures yields essential indices, expanding insight into their physical and chemical aspects. The M-polynomial hinges on vertex degrees, while the NM-polynomial builds on neighborhood degree-based indices. These tools underpin the study of prevalent biopolymers, such as xanthan gum and gellan gum [29].

A compact method to derive multiple topological indices from a single polynomial is desirable. The M-polynomial fits this criterion, and its properties shed light on degree-based topological indices. Research worldwide has applied the M-polynomial and NM-polynomial to graphene structures (see [30–34]). Recently, Mohammed Yasin et al. [29, 35] have calculated the M-polynomial and NM-polynomial concepts for biopolymer structures. In recent years, there has been a significant increase in research activity, particularly in the field of topological indices and their practical applications. Some of the most notable and widely conducted studies have focused on this area. For further details, you can refer to [36, 37].

This article's focus is calculating M-polynomial and NM-polynomial for biopolymers, generating significant indices like first and second Zagreb indices, modified second Zagreb index, third redefined Zagreb index, Forgotten index, Randic index, inverse Randic index, symmetric division index, inverse sum index, and harmonic index, along with their neighborhood variations.

3. Preliminaries

Definition 1. Let R be a simple connected graph, and the M-polynomial can be represented by the following equation:

$$M(R; x, y) = \sum_{k \le l} m_{kl}(R) x^k y^l, \tag{1}$$

where m_{kl} denotes the no. of edges $\mathrm{uv} \in E(G)$, where $d_u, d_v = k, l$, respectively, in which d_u, d_v denotes the degree of the vertices u and v in the graph, respectively.

Definition 2. Let R be a simple connected graph, and the NM-polynomial can be represented by the following equation:

$$\mathrm{NM}(R; x, y) = \sum_{k \le l} \chi_{\mathrm{kl}}(R) x^k y^l, \tag{2}$$

where χ_{kl} denotes the no. of edges $\mathrm{uv} \in E(G)$, where $\mathrm{nd}_u, \mathrm{nd}_v = k, l$, respectively, in which $\mathrm{nd}_u, \mathrm{nd}_v$ denotes the degree of the vertices u and v in the graph, respectively.

For the degree-based TIs, $\delta_u = d_u$, $\delta_v = d_v$, $p(x, y) = M(R; x, y)$, and for the neighborhood degree-based TIs, $\delta_u = \mathrm{nd}_u$, $\delta_v = \mathrm{nd}_v$, $\mathrm{NM}(R; x, y) = P(x, y)$. The degree-based and neighborhood degree-based TIs and their respective collections in the NM-polynomial and M-polynomial for graph R are tabulated in Table 1.

$$D_x = x\left(\frac{\delta(P(x,y))}{\delta x}\right), D_y = y\left(\frac{\delta(P(x,y))}{\delta y}\right), J(f(x,y)) = (p(x,y))|_{y=x},$$
$$S_x = \int_0^x \frac{p(x,y)|_{x=t}}{t}\,\mathrm{dt}, S_y = \int_0^y \frac{p(x,y)|_{y=t}}{t}\,\mathrm{dt}. \tag{3}$$

4. Methodology

Recent studies have shown that polymers could be really useful for making new medical materials. These polymers have qualities similar to regular plastics made from oil, like polypropylene. This is explained in more detail in sources ([38–40]). These natural polymers can be used for many things, similar to how we use plastics from oil, making them a good alternative. Scientists have also looked into how these polymers behave physically and how they are shaped, which is talked about in source [41]. The work deals with neighborhood degree sum-based indices for polysaccharide, poly-γ-glutamic acid, and poly-L-lysine structures. First of all, the NM-polynomials of the structures are calculated, and then, using some calculus operators, various degree sum-based indices are recovered. We use combinatorial computation, the edge partition method, and graph theoretical tools to obtain the outcomes. The graphical representations of the outcomes and comparative study of the findings are performed via 3D plotting and shown by utilizing the MATLAB software.

5. Main Results

In this part, we present our computation-based results, and we calculate M-polynomial and NM-polynomial for the biopolymers, polysaccharides, poly-γ-glutamic acid, and poly-L-lysine.

5.1. Polysaccharide. Consider a molecular graph R_1 for polysaccharide, which contains 12 n edges. m_{kl} denotes the no. of edges in which k and l denote the degree of end vertices for the set of all edges. From Figure 1, the edge partitions are given in Table 2.

χ_{kl} denotes the no. of edges in which k and l represent the neighborhood degree of end vertices for the set of all edges. From the polysaccharide structure, we obtained Table 3.

5.1.1. M-Polynomial and NM-Polynomial for Polysaccharide. Assume R_1, the molecular graph of polysaccharide.

(i) The M-polynomial for polysaccharide graph is as follows:

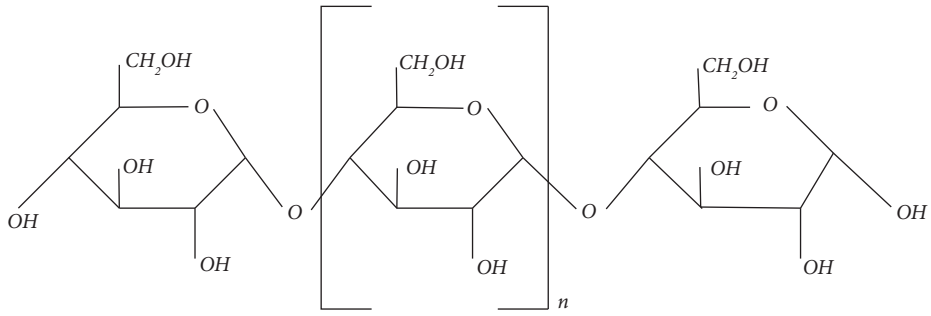
$$\begin{aligned} M(R_1; x, y) &= \sum_{k\le l} m_{\mathrm{kl}}(R) x^k y^l \\ &= |m_{1,2}|\mathrm{xy}^2 + |m_{1,3}|\mathrm{xy}^3 + |m_{2,3}|x^2y^3 + |m_{3,3}|x^3y^3 \\ &= nxy^2 + 2(n+1)\mathrm{xy}^3 + (5n-2)x^2y^3 + 4\mathrm{nx}^3y^3. \end{aligned} \tag{4}$$

(ii) The NM-polynomial for polysaccharide graph is as follows:

$$\begin{aligned} M(R_1; x, y) &= \sum_{k\le l} \chi_{\mathrm{kl}}(R) x^k y^l \\ &= |\chi_{2,4}|x^2y^4 + |\chi_{3,6}|x^3y^6 + |\chi_{3,7}|x^3y^7 + |\chi_{4,7}|x^4y^7 + |\chi_{6,6}|x^6y^6 \\ &\quad + |\chi_{6,7}|x^6y^7 + |\chi_{6,8}|x^6y^8 + |\chi_{7,7}|x^7y^7 + |\chi_{7,8}|x^7y^8 \\ &= \mathrm{nx}^2y^4 + x^3y^3 + (2n+1)x^3y^7 + \mathrm{nx}^4y^7 + x^6y^6 + (3n-1)x^6y^7 \\ &\quad + 2(n-1)x^6y^8 + (2n+1)x^7y^7 + (n-1)x^7y^8. \end{aligned} \tag{5}$$

Table 1: The correlation among several TIs with NM-polynomial and M-polynomial.

TIs	Formula $g(\delta_u, \delta_v)$	Derived from $p(x, y) = M(R; x, y)$ or $\mathrm{NM}(R; x, y)$
M_1/NM_1	$\sum_{uv\in E(G)} (\delta_u + \delta_v)$	$(D_x + D_y)(p(x, y))_{x=y=1}$
M_2/NM_2	$\sum_{uv\in E(G)} (\delta_u \times \delta_v)$	$(D_xD_y)(p(x, y))_{x=y=1}$
F/NF	$\sum_{uv\in E(G)} (\delta_u{}^2 + \delta_v{}^2)$	$(D_x{}^2 + D_y{}^2)(p(x, y))_{x=y=1}$
${}^{m}M_2/{}^{\mathrm{nm}}M_2$	$\sum_{uv\in E(G)} 1/(\delta_u.\delta_v)$	$(S_xS_y)(p(x, y))_{x=y=1}$
$R_\alpha/\mathrm{NR}_\alpha$	$\sum_{uv\in E(G)} [\delta_u\delta_v]^\alpha$	$(D_x^\alpha D_y^\alpha)(p(x, y))_{x=y=1}$
$\mathrm{ReZG}_3/\mathrm{ND}_3$	$\sum_{uv\in E(G)} (\delta_u + \delta_v)(\delta_u.\delta_v)$	$((D_xD_y)(D_x + D_y))(p(x, y))_{x=y=1}$
$\mathrm{SDD}/\mathrm{ND}_5$	$\sum_{uv\in E(G)} (\delta_{(u)}^2 + \delta_{(v)}^2/\delta_u.d\delta_v)$	$(D_xS_y + S_xD_y)(p(x, y))_{x=y=1}$
H/NH	$\sum_{uv\in E(G)} 2/\delta_u + \delta_v$	$(S_xJ)(p(x, y))_{x=y=1}$
I/NI	$\sum_{uv\in E(G)} \delta_u.\delta_v/\delta_u + \delta_v$	$(S_x\mathrm{J}D_xD_y)(p(x, y))_{x=y=1}$



Polysaccharide

Figure 1: Molecular structure of polysaccharide.

Table 2: Edge partition of the degree-based indices for polysaccharide.

(d_u, d_v), $uv \in E(G)$	No. of edges
(1, 2)	n
(1, 3)	$2n + 2$
(2, 3)	$5n - 2$
(3, 3)	$4n$

Table 3: Edge partition of the neighborhood degree-based indices for polysaccharide.

$(\mathrm{nd}_u, \mathrm{nd}_v)$, $uv \in E(G)$	No. of edges
(2, 4)	n
(3, 6)	1
(3, 7)	$2n + 1$
(4, 7)	n
(6, 6)	1
(6, 7)	$(3n - 1)$
(6, 8)	$2\ (n - 1)$
(7, 7)	$2n + 1$
(7, 8)	$n - 1$

5.1.2. Degree-Based TIs of Polysaccharide Graph Using M-Polynomial. By using equation (4), we calculated the degree-based topological indices for the polysaccharide graph, and the results are as follows:

$$\left(D_x + D_y\right)f(x, y) = 3\mathrm{nxy}^2 + 8(n + 1)\mathrm{xy}^3 + 5(5n - 2)x^2y^3 + 24\mathrm{nx}^3y^3,$$

$$\left(D_xD_y\right)f(x, y) = 2\mathrm{nxy}^2 + 6(n + 1)\mathrm{xy}^3 + 6(5n - 2)x^2y^3 + 36\mathrm{nx}^3y^3,$$

$$\left(D_x{}^2 + D_y{}^2\right)f(x, y) = 5\mathrm{nxy}^2 + 20(n + 1)\mathrm{xy}^3 + 13(5n - 2)x^2y^3 + 72\mathrm{nx}^3y^3,$$

$$\left(S_xS_y\right)f(x, y) = \frac{1}{2}\mathrm{nxy}^2 + \frac{2}{3}(n + 1)\mathrm{xy}^3 + \frac{1}{6}(5n - 2)x^2y^3 + \frac{4}{9}\mathrm{nx}^3y^3,$$

$$\begin{aligned}
\left(D_x^{\alpha}D_y^{\alpha}\right)f(x,y) &= 2^{\alpha}.\mathrm{nxy}^2 + 3^{\alpha}.2(n+1)\mathrm{xy}^3 + 6^{\alpha}(5n-2)x^2y^3 \\
&\quad + 9^{\alpha}4\mathrm{nx}^3y^3, \\
\left(\left(D_xD_y\right)\left(D_x+D_y\right)\right)f(x,y) &= 6\mathrm{nxy}^2 + 24(n+1)\mathrm{xy}^3 + 30(5n-2)x^2y^3 + 216\mathrm{nx}^3y^3, \\
\left(D_xS_y + S_xD_y\right)f(x,y) &= \frac{5}{2}\mathrm{nxy}^2 + \frac{20}{3}(n+1)\mathrm{xy}^3 + \frac{13}{6}(5n-2)x^2y^3 + 8\mathrm{nx}^3y^3, \\
\left(S_xJ\right)f(x,y) &= \frac{2}{3}\mathrm{nx}^3 + (n+1)x^4 + \frac{2}{5}(5n-2)x^5 + \frac{4}{3}\mathrm{nx}^6, \\
\left(S_x\mathrm{J}D_xD_y\right)f(x,y) &= \frac{2}{3}\mathrm{nx}^3 + \frac{3}{2}(n+1)x^4 + \frac{6}{5}(5n-2)x^5 + 6\mathrm{nx}^6. \qquad (6)
\end{aligned}$$

5.1.3. Neighborhood Degree-Based TIs of Polysaccharide Graph Using NM-Polynomial. By using equation (5), we calculated the neighborhood degree-based topological indices for the polysaccharide graph, and the results are as follows:

$$\begin{aligned}
\left(D_x+D_y\right)f(x,y) &= 6\mathrm{nx}^2y^4 + 9x^3y^6 + 10(2n+1)x^3y^7 + 11\mathrm{nx}^4y^7 + 12x^6y^6 \\
&\quad + 13(3n-1)x^6y^7 + 28(n-1)x^6y^8 + 14(2n+1)x^7y^7 \\
&\quad + 15(n-1)x^7y^8, \\
\left(D_xD_y\right)f(x,y) &= 8\mathrm{nx}^2y^4 + 18x^3y^6 + 21(2n+1)x^3y^7 + 28nx^4y^7 + 36x^6y^6 \\
&\quad + 42(3n-1)x^6y^7 + 96(n-1)x^6y^8 + 49(2n+1)x^7y^7 \\
&\quad + 56(n-1)x^7y^8, \\
\left(D_x{}^2+D_y{}^2\right)f(x,y) &= 20\mathrm{nx}^2y^4 + 45x^3y^6 + 58(2n+1)x^3y^7 + 65\mathrm{nx}^4y^7 + 72x^6y^6 \\
&\quad + 85(3n-1)x^6y^7 + 200(n-1)x^6y^8 + 98(2n+1)x^7y^7 \\
&\quad + 113(n-1)x^7y^8, \\
\left(S_xS_y\right)f(x,y) &= \frac{1}{8}nx^2y^4 + \frac{1}{18}x^3y^6 + \frac{1}{21}(2n+1)x^3y^7 + \frac{1}{28}\mathrm{nx}^4y^7 \\
&\quad + \frac{1}{36}x^6y^6 + \frac{1}{42}(3n-1)x^6y^7 + \frac{1}{24}(n-1)x^6y^8 \\
&\quad + \frac{1}{49}(2n+1)x^7y^7 + \frac{1}{56}(n-1)x^7y^8, \\
\left(D_x^{\alpha}D_y^{\alpha}\right)f(x,y) &= 8^{\alpha}\mathrm{nx}^2y^4 + 18^{\alpha}x^3y^6 + 21^{\alpha}(2n+1)x^3y^7 + 28^{\alpha}\mathrm{nx}^4y^7 \\
&\quad + 36^{\alpha}x^6y^6 + 42^{\alpha}(3n-1)x^6y^7 + 48^{\alpha}2(n-1)x^6y^8 \\
&\quad + 49^{\alpha}(2n+1)x^7y^7 + 56^{\alpha}(n-1)x^7y^8, \\
\left(\left(D_xD_y\right)\left(D_x+D_y\right)\right)f(x,y) &= 48\mathrm{nx}^2y^4 + 162x^3y^6 + 210(2n+1)x^3y^7 + 308\mathrm{nx}^4y^7 \\
&\quad + 432x^6y^6 + 546(3n-1)x^6y^7 + 1344(n-1)x^6y^8 \\
&\quad + 686(2n+1)x^7y^7 + 840(n-1)x^7y^8,
\end{aligned}$$

$$\begin{aligned}
\left(D_xS_y + S_xD_y\right)f(x,y) &= \frac{5}{2}\mathrm{n}x^2y^4 + \frac{5}{2}x^3y^6 + \frac{58}{21}(2n+1)x^3y^7 + \frac{65}{28}\mathrm{n}x^4y^7 + 2x^6y^6 \\
&\quad + \frac{85}{42}(3n-1)x^6y^7 + \frac{25}{6}(n-1)x^6y^8 + 2(2n+1)x^7y^7 \\
&\quad + \frac{113}{56}(n-1)x^7y^8, \\
(S_xJ)f(x,y) &= \frac{1}{3}\mathrm{n}x^6 + \frac{2}{9}x^9 + \frac{1}{5}(2n+1)x^{10} + \frac{2}{11}\mathrm{n}x^{11} + \frac{1}{6}x^{12} \\
&\quad + \frac{2}{13}(3n-1)x^{13} + \frac{1}{7}(4n-1)x^{14} + \frac{2}{15}(n-1)x^{15}, \\
\left(S_x\mathrm{JD}_xD_y\right)f(x,y) &= \frac{4}{3}\mathrm{n}x^6 + 2x^9 + \frac{21}{10}(2n+1)x^{10} + \frac{28}{11}\mathrm{n}x^{11} + 3x^{12} \\
&\quad + \frac{42}{13}(3n-1)x^{13} + \frac{1}{14}(194n-47)x^{14} + \frac{56}{15}(n-1)x^{15}.
\end{aligned} \tag{7}$$

Now, by the help of partition of edges for poly-γ-glutamic acid and poly-L-lysine, the same method is used to prove M-polynomial and NM-polynomial for polysaccharide which can be utilized to prove for poly-γ-glutamic acid and poly-L-lysine.

We narrow few degree-based and neighborhood degree-based TIs of poly-γ-glutamic acid and poly-L-lysine, with the help of the M-polynomial and NM-polynomial with the identical usage of polysaccharide.

5.2. Poly-γ-glutamic Acid. Consider R_2, the graph of poly-γ-glutamic acid which contains 9 n edges. From Figure 2, the partition of edges according to vertex degrees is tabulated in Table 4.

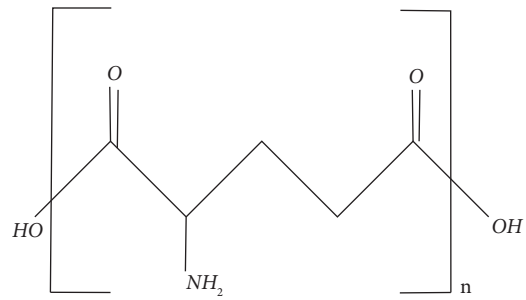
Also, the partition of edges according to neighborhood degree sum vertices is shown in Table 5.

5.2.1. M-Polynomial and NM-Polynomial for Poly-γ-glutamic Acid. Assume R_2, the molecular graph of poly-γ-glutamic acid. The M-polynomial and NM-polynomial for poly-γ-glutamic acid are as follows:

$$M(R_2,x,y) = (3n+2)\mathrm{x}y^3 + \mathrm{n}x^2y^2 + (4n-2)x^2y^3 + \mathrm{n}x^3y^3, \tag{8}$$

$$\begin{aligned}
\mathrm{NM}(R_2,x,y) &= 2x^3y^4 + 2\mathrm{n}x^3y^5 + (2n-1)x^3y^6 + x^4y^5 + (2n-1)x^5y^5 \\
&\quad + (n+1)x^5y^6 + 2\mathrm{n}x^6y^6.
\end{aligned} \tag{9}$$

5.2.2. Degree-Based TIs of Poly-γ-glutamic Acid Graph Using M-Polynomial. By using equation (8), we calculated the degree-based topological indices for the poly-γ-glutamic acid graph, and the results are as follows:



Poly-γ-Glutamic acid

Figure 2: Molecular structure of poly-γ-glutamic acid.

Table 4: Edge partition of the degree-based indices for poly-γ-glutamic acid.

(d_u, d_v), uv ∈ $E(G)$	No. of edges
(1, 3)	$3n+2$
(2, 2)	n
(2, 3)	$4n-2$
(3, 3)	n

Table 5: Edge partition of the neighborhood degree-based indices for poly-γ-glutamic acid.

$(\mathrm{nd}_u, \mathrm{nd}_u)$, uv ∈ $E(G)$	No. of edges
(3, 4)	2
(3, 5)	$2n$
(3, 6)	$2n-1$
(4, 5)	1
(5, 5)	$2n-1$
(5, 6)	$n+1$
(6, 6)	$2n$

$$
\begin{aligned}
\left(D_x + D_y\right) f(x,y) &= 4(3n+2)\mathrm{xy}^3 + 4\mathrm{nx}^2y^2 + 5(4n-2)x^2y^3 + 6\mathrm{nx}^3y^3,\\
\left(D_xD_y\right) f(x,y) &= 3(3n+2)\mathrm{xy}^3 + 4\mathrm{nx}^2y^2 + 6(4n-2)x^2y^3 + 9\mathrm{nx}^3y^3,\\
\left({D_x}^2 + {D_y}^2\right) f(x,y) &= 10(3n+2)\mathrm{xy}^3 + 8\mathrm{nx}^2y^2 + 13(4n-2)x^2y^3 + 18\mathrm{nx}^3y^3,\\
\left(S_xS_y\right) f(x,y) &= \frac{1}{3}(3n+2)\mathrm{xy}^3 + \frac{1}{4}\mathrm{nx}^2y^2 + \frac{1}{6}(4n-2)x^2y^3 + \frac{1}{9}\mathrm{nx}^3y^3,\\
\left(D_x^{\alpha}D_y^{\alpha}\right) f(x,y) &= 3^{\alpha}.(3n+2)\mathrm{xy}^3 + 4^{\alpha}.\mathrm{nx}^2y^2 + 6^{\alpha}(4n-2)x^2y^3 + 9^{\alpha}\mathrm{nx}^3y^3,\\
\left(\left(D_xD_y\right)\left(D_x + D_y\right)\right) f(x,y) &= 12(3n+2)\mathrm{xy}^3 + 16\mathrm{nx}^2y^2 + 30(4n-2)x^2y^3 + 54\mathrm{nx}^3y^3,\\
\left(D_xS_y + S_xD_y\right) f(x,y) &= \frac{10}{3}(3n+2)\mathrm{xy}^3 + 2\mathrm{nx}^2y^2 + \frac{13}{6}(4n-2)x^2y^3 + 2\mathrm{nx}^3y^3,\\
\left(S_xJ\right) f(x,y) &= (2n+1)x^4 + \frac{2}{5}(4n-2)x^5 + \frac{1}{3}\mathrm{nx}^6,\\
\left(S_x\mathrm{J}D_xD_y\right) f(x,y) &= \frac{1}{4}(13n+6)x^4 + \frac{6}{5}(4n-2)x^5 + \frac{3}{2}\mathrm{nx}^6.
\end{aligned}
\tag{10}
$$

5.2.3. Neighborhood Degree-Based TIs of Poly-γ-glutamic Acid Graph Using NM-Polynomial. By using equation (9), we calculated the neighborhood degree-based topological indices for the poly-γ-glutamic acid graph, and the results are as follows:

$$
\begin{aligned}
\left(D_x + D_y\right) f(x,y) &= 14x^3y^4 + 16\mathrm{n}x^3y^5 + 9(2n-1)x^3y^6 + 9x^4y^5 \\
&\quad + 10(2n-1)x^5y^5 + 11(n+1)x^5y^6 + 24\mathrm{n}x^6y^6, \\
\left(D_xD_y\right) f(x,y) &= 24x^3y^4 + 30\mathrm{n}x^3y^5 + 18(2n-1)x^3y^6 + 20x^4y^5 \\
&\quad + 25(2n-1)x^5y^5 + 30(n+1)x^5y^6 + 72\mathrm{n}x^6y^6, \\
\left(D_x{}^2 + D_y{}^2\right) f(x,y) &= 50x^3y^4 + 68\mathrm{n}x^3y^5 + 45(2n-1)x^3y^6 + 41x^4y^5 \\
&\quad + 50(2n-1)x^5y^5 + 61(n+1)x^5y^6 + 144\mathrm{n}x^6y^6, \\
\left(S_xS_y\right) f(x,y) &= \frac{1}{6}x^3y^4 + \frac{2}{15}\mathrm{n}x^3y^5 + \frac{1}{18}(2n-1)x^3y^6 + \frac{1}{20}x^4y^5 \\
&\quad + \frac{1}{25}(2n-1)x^5y^5 + \frac{1}{30}(n+1)x^5y^6 + \frac{1}{18}\mathrm{n}x^6y^6, \\
\left(D_x^{\alpha}D_y^{\alpha}\right) f(x,y) &= 12^{\alpha}2x^3y^4 + 15^{\alpha}2\mathrm{n}x^3y^5 + 18^{\alpha}(2n-1)x^3y^6 + 20^{\alpha}x^4y^5 \\
&\quad + 25^{\alpha}(2n-1)x^5y^5 + 30^{\alpha}(n+1)x^5y^6 + 36^{\alpha}2\mathrm{n}x^6y^6, \\
\left(\left(D_xD_y\right)\left(D_x + D_y\right)\right) f(x,y) &= 168x^3y^4 + 240\mathrm{n}x^3y^5 + 162(2n-1)x^3y^6 + 180x^4y^5 \\
&\quad + 250(2n-1)x^5y^5 + 330(n+1)x^5y^6 + 864\mathrm{n}x^6y^6, \\
\left(D_xS_y + S_xD_y\right) f(x,y) &= \frac{25}{6}x^3y^4 + \frac{68}{15}\mathrm{n}x^3y^5 + \frac{5}{2}(2n-1)x^3y^6 + \frac{41}{20}x^4y^5 \\
&\quad + 2(2n-1)x^5y^5 + \frac{61}{30}(n+1)x^5y^6 + 4\mathrm{n}x^6y^6, \\
\left(S_xJ\right) f(x,y) &= \frac{4}{7}x^7 + \frac{1}{2}\mathrm{n}x^8 + \frac{4}{9}\mathrm{n}x^9 + \frac{1}{5}(2n-1)x^{10} + \frac{2}{11}(n+1)x^{11} \\
&\quad + \frac{1}{3}\mathrm{n}x^{12}, \\
\left(S_x\mathrm{J}D_xD_y\right) f(x,y) &= \frac{24}{7}x^7 + \frac{15}{4}\mathrm{n}x^8 + 2(2n-1)x^9 + \frac{20}{9}x^9\frac{5}{2}(2n-1)x^{10} \\
&\quad + \frac{30}{11}(n+1)x^{11} + 6\mathrm{n}x^{12}.
\end{aligned}
\tag{11}
$$

5.3. Poly-L-lysine. Consider R_3, the graph of poly-l-lysine which has 10n edges. From Figure 3, the partition of edges according to vertex degrees is tabulated in Table 6.

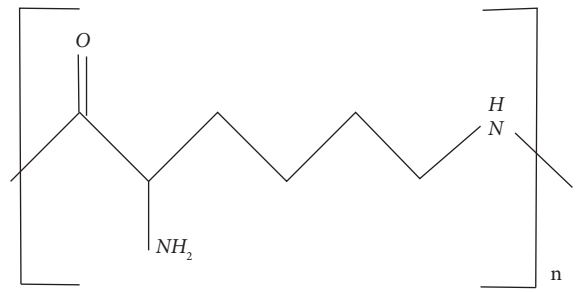
Also, the partition of edges according to neighborhood degree sum vertices is shown in Table 7.

5.3.1. M-Polynomial and NM-Polynomial for Poly-L-lysine. Assume R_3, the molecular graph of poly-L-lysine. The M-polynomial and NM-polynomial for poly-L-lysine are as follows:

$$
M(R_3, x, y) = \mathrm{x}y^2 + (2n+1)\mathrm{x}y^3 + (5n-1)x^2y^2 + (2n-1)x^2y^3 + \mathrm{n}x^3y^3, \tag{12}
$$

$$
\begin{aligned}
\mathrm{NM}(R_3, x, y) &= x^2y^3 + x^3y^4 + 2x^3y^5 + (2n-1)x^3y^6 + (3n-1)x^4y^4 + (2n-1)x^4y^5 \\
&\quad + (3n-1)x^5y^6.
\end{aligned}
\tag{13}
$$

5.3.2. Degree-Based TIs of Poly-L-lysine Graph Using M-Polynomial. By using equation (12), we calculated the degree-based topological indices for the poly-L-lysine graph, and the results are as follows:



Poly-L-lysine

Figure 3: Molecular structure of poly-L-lysine.

Table 6: Edge partition of degree-based indices for poly-L-lysine.

(d_u, d_v), uv $\in E(G)$	No. of edges
(1, 2)	1
(1, 3)	$2n+1$
(2, 2)	$5n-1$
(2, 3)	$2n-1$
(3, 3)	n

Table 7: Edge partition of neighborhood degree-based indices for poly-L-lysine

$(\mathrm{nd}_u, \mathrm{nd}_v)$, uv $\in E(G)$	No. of edges
(2, 3)	1
(3, 4)	1
(3, 5)	2
(3, 6)	$2n-1$
(4, 4)	$3n-1$
(4, 5)	$2n-1$
(5, 6)	$3n-1$

$$
\begin{aligned}
\left(D_x + D_y\right) f(x,y) &= 3\mathrm{xy}^2 + 4(2n+1)\mathrm{xy}^3 + 4(5n-1)x^2y^2 + 5(2n-1)x^2y^3 \\
&\quad + 6\mathrm{nx}^3y^3, \\
\left(D_xD_y\right) f(x,y) &= 2\mathrm{xy}^2 + 3(2n+1)\mathrm{xy}^3 + 4(5n-1)x^2y^2 + 6(2n-1)x^2y^3 \\
&\quad + 9\mathrm{nx}^3y^3, \\
\left({D_x}^2 + {D_y}^2\right) f(x,y) &= 5\mathrm{xy}^2 + 10(2n+1)\mathrm{xy}^3 + 8(5n-1)x^2y^2 + 13(2n-1)x^2y^3 \\
&\quad + 18\mathrm{nx}^3y^3, \\
\left(S_xS_y\right) f(x,y) &= \frac{1}{2}\mathrm{xy}^2 + \frac{1}{3}(2n+1)\mathrm{xy}^3 + \frac{1}{4}(5n-1)x^2y^2 + \frac{1}{6}(2n-1)x^2y^3 \\
&\quad + \frac{1}{9}\mathrm{nx}^3y^3, \\
\left(D_x^{\alpha}D_y^{\alpha}\right) f(x,y) &= 2^{\alpha}\mathrm{xy}^2 + 3^{\alpha}.(2n+1)\mathrm{xy}^3 + 4^{\alpha}(5n-1)x^2y^3 + 6^{\alpha}(2n-1)x^2y^3 \\
&\quad + 9^{\alpha}\mathrm{nx}^3y^3, \\
\left(\left(D_xD_y\right)\left(D_x + D_y\right)\right) f(x,y) &= 6\mathrm{xy}^2 + 12(2n+1)\mathrm{xy}^3 + 16(5n-1)x^2y^2 \\
&\quad + 30(2n-1)x^2y^3 + 54\mathrm{nx}^3y^3, \\
\left(D_xS_y + S_xD_y\right) f(x,y) &= \frac{5}{2}\mathrm{xy}^2 + \frac{10}{3}(2n+1)\mathrm{xy}^3 + 2(5n-1)x^2y^2 \\
&\quad + \frac{13}{6}(2n-1)x^2y^3 + 2\mathrm{nx}^3y^3, \\
\left(S_xJ\right) f(x,y) &= \frac{2}{3}x^3 + \frac{7}{2}\mathrm{nx}^4 + \frac{2}{5}(2n-1)x^5 + \frac{1}{3}\mathrm{nx}^6, \\
\left(S_x\mathrm{J}D_xD_y\right) f(x,y) &= \frac{1}{3}x^3 + \frac{1}{2}\left(13n - \frac{1}{2}\right)x^4 + \frac{6}{5}(2n-1)x^5 + \frac{3}{2}\mathrm{nx}^6.
\end{aligned}
\tag{14}
$$

5.3.3. Neighborhood Degree-Based TIs of Poly-L-lysine Graph Using NM-Polynomial. By using equation (13), we calculated the neighborhood degree-based topological indices for the poly-L-lysine graph, and the results are as follows:

$$
\begin{aligned}
\left(D_x + D_y\right) f(x,y) &= 5x^2y^3 + 7x^3y^4 + 16x^3y^5 + 9(2n-1)x^3y^6 + 8(3n-1)x^4y^4 \\
&\quad + 9(2n-1)x^4y^5 + 11(3n-1)x^5y^6, \\
\left(D_xD_y\right) f(x,y) &= 6x^2y^3 + 12x^3y^4 + 30x^3y^5 + 18(2n-1)x^3y^6 \\
&\quad + 16(3n-1)x^4y^4 + 20(2n-1)x^4y^5 + 30(3n-1)x^5y^6, \\
\left(D_x{}^2 + D_y{}^2\right) f(x,y) &= 13x^2y^3 + 25x^3y^4 + 68x^3y^5 + 45(2n-1)x^3y^6 \\
&\quad + 32(3n-1)x^4y^4 + 41(2n-1)x^4y^5 + 61(3n-1)x^5y^6, \\
\left(S_xS_y\right) f(x,y) &= \frac{1}{6}x^2y^3 + \frac{1}{12}x^3y^4 + \frac{2}{15}x^3y^5 + \frac{1}{18}(2n-1)x^3y^6 \\
&\quad + \frac{1}{16}(3n-1)x^4y^4 + \frac{1}{20}(2n-1)x^4y^5 + \frac{1}{30}(3n-1)x^5y^6, \\
\left(D_x^{\alpha}D_y^{\alpha}\right) f(x,y) &= 6^{\alpha}x^2y^3 + 12^{\alpha}x^3y^4 + 15^{\alpha}2x^3y^5 + 18^{\alpha}(2n-1)x^3y^6 \\
&\quad + 16^{\alpha}(3n-1)x^4y^4 + 20^{\alpha}(2n-1)x^4y^5 \\
&\quad + 30^{\alpha}(3n-1)x^5y^6, \\
\left(\left(D_xD_y\right)\left(D_x + D_y\right)\right) f(x,y) &= 30x^2y^3 + 84x^3y^4 + 240x^3y^5 + 162(2n-1)x^3y^6 \\
&\quad + 128(3n-1)x^4y^4 + 180(2n-1)x^4y^5 \\
&\quad + 330(3n-1)x^5y^6, \\
\left(D_xS_y + S_xD_y\right) f(x,y) &= \frac{13}{6}x^2y^3 + \frac{25}{12}x^3y^4 + \frac{68}{15}x^3y^5 + \frac{5}{2}(2n-1)x^3y^6 \\
&\quad + 2(3n-1)x^4y^4 + \frac{41}{20}(2n-1)x^4y^5 + \frac{61}{30}(3n-1)x^5y^6, \\
\left(S_xJ\right) f(x,y) &= \frac{2}{5}x^5 + \frac{2}{7}x^7 + \frac{1}{4}(3n-1)x^8 + \frac{4}{9}(2n-1)x^9 \\
&\quad + \frac{2}{11}(3n-1)x^{11}, \\
\left(S_x\mathrm{J}D_xD_y\right) f(x,y) &= \frac{6}{5}x^5 + \frac{12}{7}x^7 + \frac{1}{8}(48n-1)x^8 + \frac{38}{9}(2n-1)x^9 \\
&\quad + \frac{30}{11}(3n-1)x^{11}.
\end{aligned}
\tag{15}
$$

Both the M-polynomial and the NM-polynomial, respectively, are replete with details on neighborhood degree-based and degree-based TIs. We believe further investigation of the properties of M-polynomials and NM-polynomials will result in newer, all-encompassing generalizations in the study of TIs. To view the polynomials, MATLAB does surface plotting. Figures 4–6 show the graphic representations for the M-polynomials and the NM-polynomials. Utilizing the x and y parameters, we first make a horizontal grid, and we construct a surface on the head of that grid. Depending on the parameters, these graphs show various features of the polynomials. By manipulating polynomials through these parameters, we can exert control over various aspects and activities. For the significance of Tables 8–13, we show the graphical representation for value comparison of various degree-based and neighborhood degree-based topological indices of polysaccharide, poly-γ-glutamic acid, and poly-L-lysine, respectively, in Figures 7–9. In this study, "n" represents the number of molecular structures, ranging approximately from 1 to 10.

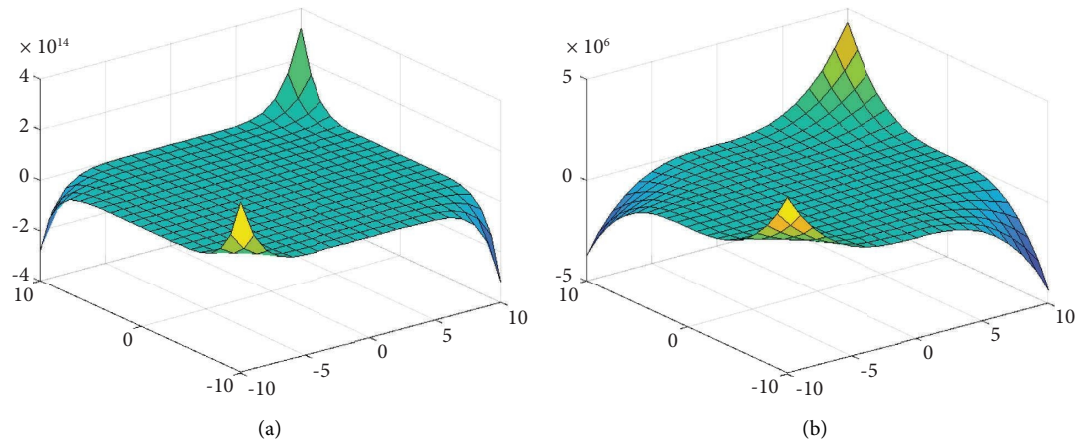


Figure 4: 3D plot representation of (a) NM-polynomial in equation (5) and (b) M-polynomial in equation (4) of polysaccharide molecular graph.

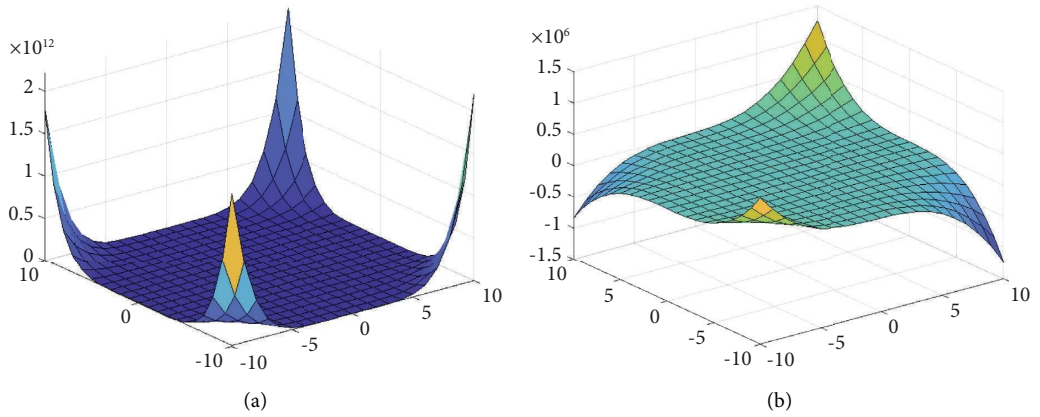


Figure 5: 3D plot representation of (a) NM-polynomial in equation (8) and (b) M-polynomial in equation (9) of poly-γ-glutamic acid molecular graph.

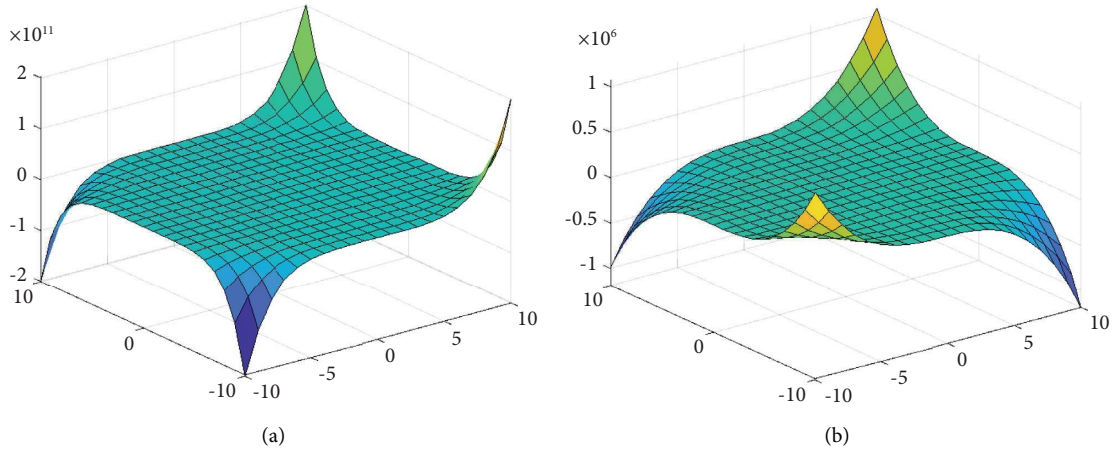


Figure 6: 3D plot representation of (a) NM-polynomial in equation (12) and (b) M-polynomial in equation (13) of poly-L-lysine molecular graph.

Table 8: Numerical comparison of degree-based indices of polysaccharide for $n = 1$ to 10.

$[n]$	M_1	M_2	F	${}^{m}M_2$	R	ReZG_3	SDD	H	I
1	58	68	156	2.78	5.57	360	30.33	5.2	12.77
2	118	142	318	5.22	10.81	756	58.33	10.2	26.93
3	178	216	480	7.67	16.05	1152	86.33	15.2	41.10
4	238	290	642	10.11	21.28	1548	114.33	20.2	55.27
5	298	364	804	12.56	26.52	1944	142.33	25.2	69.43
6	358	438	966	15.00	31.76	2340	170.33	30.2	83.60
7	418	512	1128	17.44	36.99	2736	198.33	35.2	97.77
8	478	586	1290	19.89	42.23	3132	226.33	40.2	111.93
9	538	660	1452	22.33	47.47	3528	254.33	45.2	126.10
10	598	734	1614	24.78	52.70	3924	282.33	50.2	140.27

Table 9: Numerical comparison of neighborhood degree-based indices of polysaccharide for $n = 1$ to 10.

$[n]$	NM_1	NM_2	NF	${}^{nm}\mathrm{NM}_2$	NR	ND_3	ND_5	NH	NI
1	136	384	840	0.50	2.34	4730	27.65	2.24	32.14
2	283	838	1805	0.92	4.49	10700	54.26	4.32	67.50
3	430	1292	2770	1.35	6.64	16670	80.86	6.40	102.86
4	577	1746	3735	1.78	8.79	22640	107.46	8.48	138.23
5	724	2200	4700	2.21	10.94	28610	134.06	10.57	173.59
6	871	2654	5665	2.63	13.09	34580	160.66	12.65	208.95
7	1018	3108	6630	3.06	15.24	40550	187.26	14.73	244.31
8	1165	3562	7595	3.49	17.39	46520	213.86	16.81	279.67
9	1312	4016	8560	3.92	19.54	52490	240.46	18.89	315.03
10	1459	4470	9525	4.35	21.69	58460	267.07	20.97	350.39

Table 10: Numerical comparison of degree-based indices of poly-γ-glutamic acid for $n = 1$ to 10.

$[n]$	M_1	M_2	F	${}^{m}M_2$	R	ReZG_3	SDD	H	I
1	40	40	102	2.36	4.54	190	25.00	4.13	8.65
2	82	86	210	4.39	8.73	416	47.67	8.07	18.20
3	124	132	318	6.42	12.93	642	70.33	12.00	27.75
4	166	178	426	8.44	17.13	868	93.00	15.93	37.30
5	208	224	534	10.47	21.33	1094	115.93	19.87	46.85
6	250	270	642	12.50	25.53	1320	138.33	23.80	56.40
7	292	316	750	14.53	29.73	1546	161.00	27.73	65.95
8	334	362	858	16.56	33.93	1772	183.67	31.67	75.50
9	376	408	966	18.58	38.12	1998	206.33	35.60	85.05
10	418	454	1074	20.61	42.32	2224	229.00	39.53	94.60

Table 11: Numerical comparison of neighborhood degree-based indices of poly-γ-glutamic acid for $n = 1$ to 10.

$[n]$	NM_1	NM_2	NF	${}^{nm}\mathrm{NM}_2$	NR	ND_3	ND_5	NH	NI
1	104	249	520	0.57	2.45	2524	23.32	2.28	26.13
2	193	467	983	0.98	4.36	4782	42.88	3.87	47.61
3	282	685	1446	1.39	6.26	7040	62.45	5.47	69.09
4	371	903	1909	1.81	8.16	9298	82.02	7.06	90.56
5	460	1121	2372	2.22	10.07	11556	101.58	8.65	112.04
6	549	1339	2835	2.63	11.97	13814	121.15	10.24	133.52
7	638	1557	3298	3.05	13.87	16072	140.72	11.84	155.00
8	727	1775	3761	3.46	15.78	18330	160.28	13.43	176.47
9	816	1993	4224	3.87	17.68	20588	179.85	15.02	197.95
10	905	2211	4687	4.29	19.58	22846	199.42	16.62	219.43

Table 12: Numerical comparison of degree-based indices of poly-L-lysine for $n = 1$ to 10.

$[n]$	M_1	M_2	F	${}^{m}M_2$	R	$ReZG_3$	SDD	H	I
1	42	42	78	2.78	5.18	190	24.67	4.90	12.41
2	86	89	154	5.14	9.99	408	47.67	9.53	26.06
3	130	136	230	7.50	14.79	626	70.67	14.17	39.71
4	174	183	306	9.86	19.59	844	93.67	18.80	53.36
5	218	230	382	12.22	24.40	1062	116.67	23.43	67.01
6	262	277	458	14.58	29.20	1280	139.67	28.07	80.66
7	306	324	534	16.94	34.01	1498	162.67	32.70	94.31
8	350	371	610	19.31	38.81	1716	185.67	37.33	107.96
9	394	418	686	21.67	43.62	1934	208.67	41.97	121.67
10	438	465	762	24.03	48.42	2152	231.67	46.60	135.26

Table 13: Numerical comparison of neighborhood degree-based indices of poly-L-lysine for $n = 1$ to 10.

$[n]$	NM_1	NM_2	NF	${}^{nm}NM_2$	NR	ND_3	ND_5	NH	NI
1	84	178	378	0.68	2.54	1612	21.40	1.99	18.47
2	177	392	829	1.18	4.75	3670	42.60	4.18	41.09
3	270	606	1280	1.68	6.97	5278	63.80	6.36	63.72
4	363	820	1731	2.18	9.19	7786	85.00	8.55	86.34
5	456	1034	2182	2.68	11.40	9844	106.20	10.73	108.97
6	549	1248	2633	3.17	13.62	11902	127.40	12.92	131.60
7	642	1462	3084	3.67	15.84	13960	148.60	15.10	154.22
8	735	1676	3535	4.17	18.05	16018	169.80	17.28	176.85
9	828	1890	3986	4.67	20.27	18076	191.00	19.47	199.48
10	921	2104	4437	5.17	22.48	20134	212.20	21.65	222.10

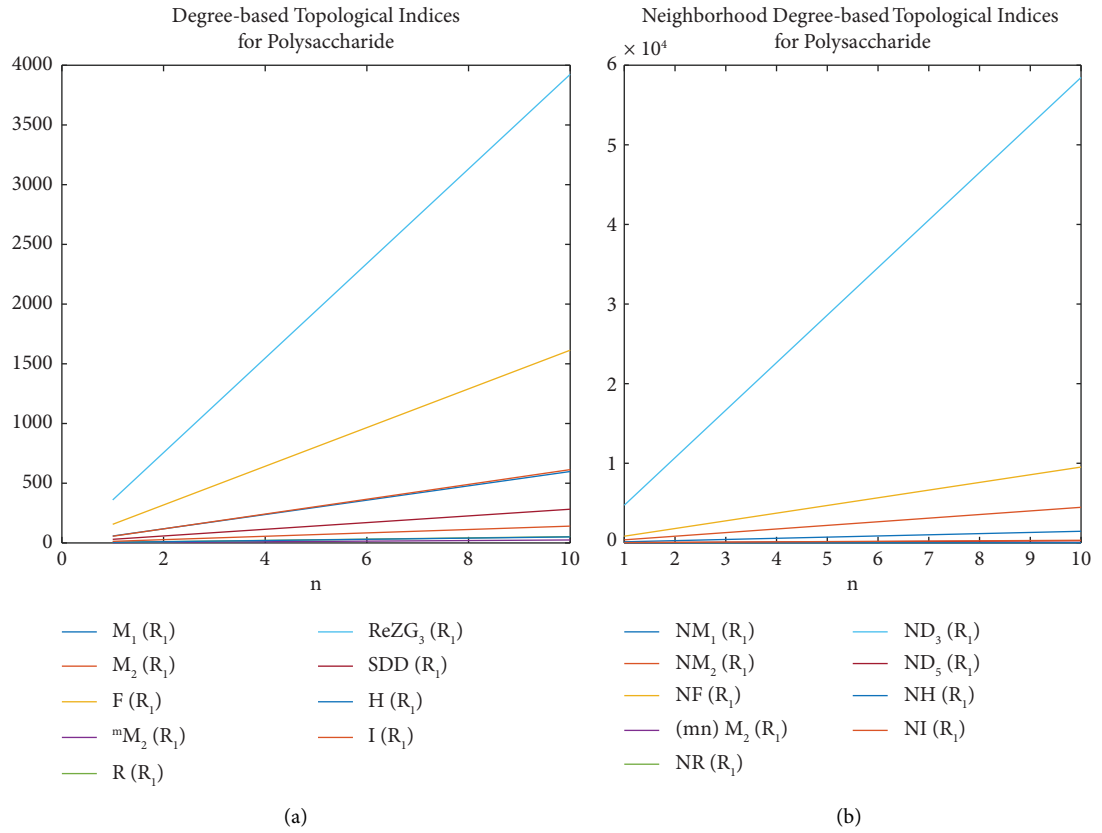


Figure 7: Graphical representation of (a) degree-based TIs and (b) neighborhood degree-based TIs for polysaccharide graph.

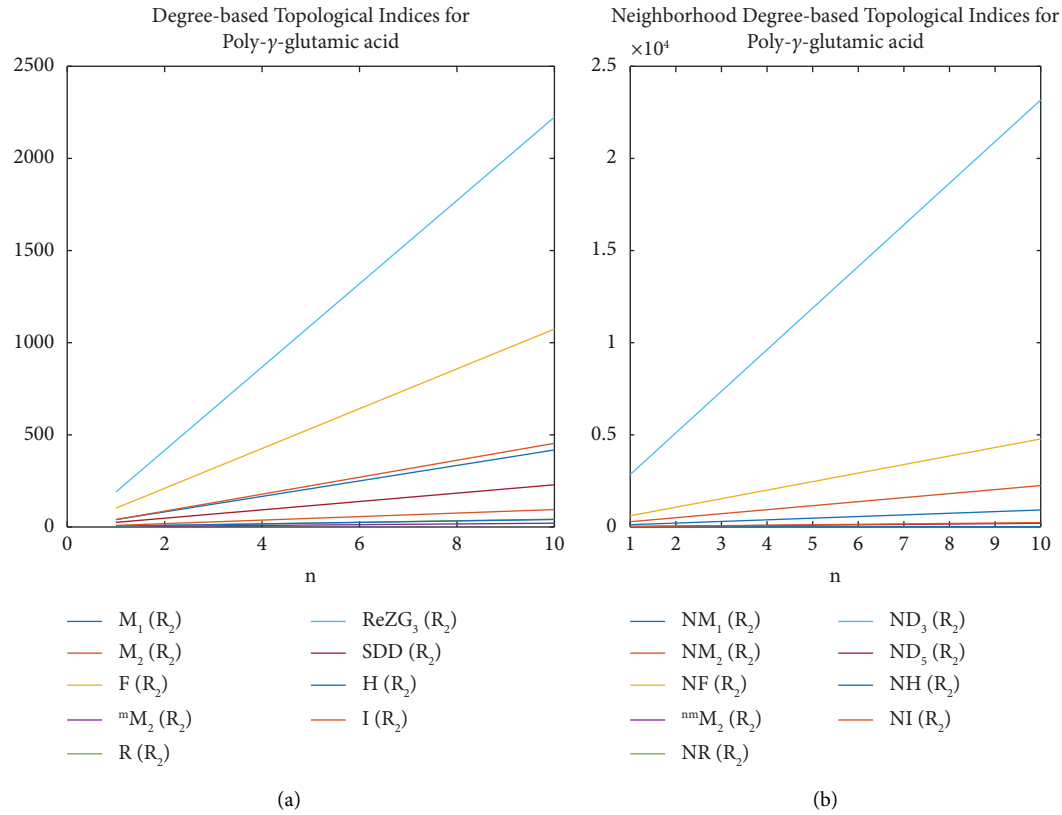


Figure 8: Graphical representation of (a) degree-based TIs and (b) neighborhood degree-based TIs for poly-γ-glutamic acid graph.

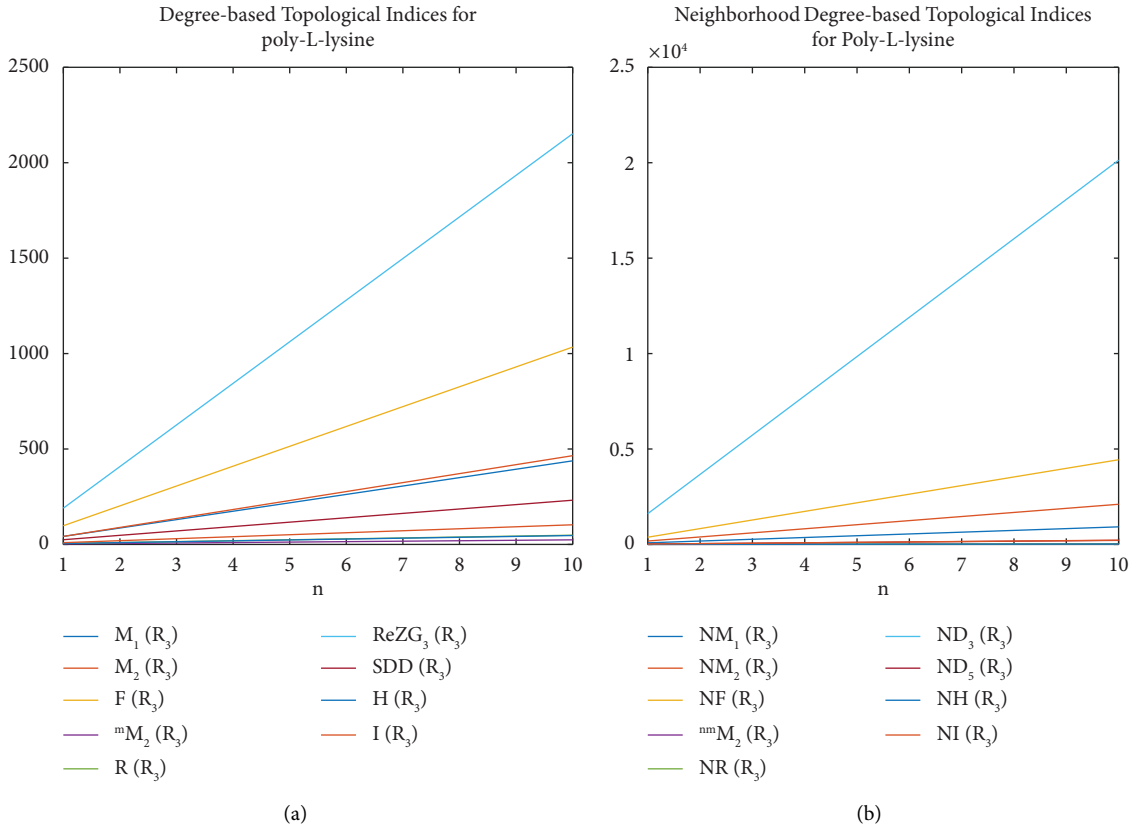


Figure 9: Graphical representation of (a) degree-based TIs and (b) neighborhood degree-based TIs for poly-L-lysine graph.

6. Numerical and Graphical Comparison of the Indices

In Section 4, various degree-based and neighborhood degree-based TIs are calculated for the polymers, including polysaccharide, poly-γ-glutamic acid, and poly-L-lysine molecular graphs using M-polynomial and NM-polynomial methods. To verify the behavior of indices, different values of n are considered. It is noticed from Tables 8–13 that the values of TIs increases as the n value increases. The behaviors of the M-polynomial and NM-polynomial are shown in Figures 4–6. The obtained TIs are represented using graphs for the distinct values of n as shown in Figures 7–9. The variation of values of degree-based and neighborhood degree-based indices is observed, and the following points are noted. In degree-based indices of polysaccharide poly-γ-glutamic acid and poly-L-lysine graphs from Tables 8, 10, and 12, it is observed that $\mathrm{ReZG}_3 > F > M_2 > M_1 > \mathrm{SDD} > I > R > H > {}^{m}M_2$. It is obvious that ReZG_3 is the highest numerical value and ${}^{m}M_2$ is the least value for every value of $n = 1$ to 10 among all the nine degree-based indices considered in this study. Similarly, by observing Tables 9, 11, and 13, the neighborhood degree-based indices for the graphs observe that $\mathrm{ND}_3 > \mathrm{NF} > \mathrm{NM}_2 > \mathrm{NM}_1 > \mathrm{ND}_5 > \mathrm{NI} > \mathrm{NR} > \mathrm{NH} > {}^{m}\mathrm{NM}_2$. It is obvious that ND_3 is the highest numerical and ${}^{m}\mathrm{NM}_2$ is the lowest value for every value of $n = 1$ to 10 among all the nine neighborhood indices considered in this study.

To clarify the physical significance of our results and the effectiveness of the computed topological indices, we have added concise discussions. These indices numerically capture key structural aspects of our studied polymers. Higher values often correspond to enhanced stability and lower reactivity, while lower values indicate potential reactivity sites. The strong correlation between certain indices and experimentally measured properties validates their predictive power. Our study underscores their utility in designing polymers for drug delivery and tailored material properties. We also acknowledge the need for considering molecular context and exploring advanced methods for even greater accuracy. These insights advance our understanding of polymer structure-property relationships.

7. Conclusion

The paper examines various topological indices, including the first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$, modified second Zagreb index ${}^{m}M_2(G)$, third redefined Zagreb index $\mathrm{ReZG}_3(G)$, forgotten index $F(G)$, Randic index $R(G)$, inverse Randic index $\mathrm{RR}(G)$, symmetric division index $\mathrm{SDD}(G)$, inverse sum index $I(G)$, harmonic index $H(G)$ and its neighborhood versions of the above indices for the polysaccharide, poly-γ-glutamic acid, and poly-L-lysine structures. The M-polynomials and NM-polynomials of the aforementioned structures are calculated to create few degree-based and neighborhood degree sum-based indices, and graphical representations are also composed for these polynomials. In the future, the work aims to correlate the physicochemical features of distinct chemical compounds to the forecasting power of neighborhood degree-based TIs.

Data Availability

The data used to support the findings of this study are cited at relevant places within the text as references.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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References

[1] M. Chamua, R. Moran, A. Pegu, and A. Bharali, "M-polynomial and neighborhood M-polynomial of some concise drug structures: azacitidine, Decitabine and Guadecitabine," *Journal of Molecular Structure*, vol. 1263, Article ID 133197, 2022.

[2] M. C. Shanmukha, A. Usha, K. C. Shilpa, and N. S. Basavarajappa, "M-polynomial and neighborhood M-polynomial methods for topological indices of porous graphene," *The European Physical Journal Plus*, vol. 136, pp. 1089–1116, 2021.

[3] S. Mondal, M. K. Siddiqui, N. De, and A. Pal, "Neighborhood M-polynomial of crystallographic structures," *Biointerface Research in Applied Chemistr*, vol. 11, pp. 9372–9381, 2021.

[4] Ö. Ç. Havare, "Topological indices and QSPR modeling of some novel drugs used in the cancer treatment," *International Journal of Quantum Chemistry*, vol. 121, no. 24, Article ID e26813, 2021.

[5] S. Mondal, N. De, and A. Pal, "Topological indices of some chemical structures applied for the treatment of COVID-19 patients," *Polycyclic Aromatic Compounds*, vol. 42, no. 4, pp. 1220–1234, 2022.

[6] S. Mondal, M. Imran, N. De, and A. Pal, "Neighborhood M-polynomial of titanium compounds," *Arabian Journal of Chemistry*, vol. 14, no. 8, Article ID 103244, 2021.

[7] P. Prasher, M. Sharma, M. Mehta et al., "Current-status and applications of polysaccharides in drug delivery systems," *Colloid and Interface Science Communications*, vol. 42, Article ID 100418, 2021.

[8] O. A. Balogun-Agbaje, O. A. Odeniyi, and M. A. Odeniyi, "Drug delivery applications of poly-γ-glutamic acid," *Future Journal of Pharmaceutical Sciences*, vol. 7, no. 1, pp. 1–10, 2021.

[9] D. Mazia, G. Schatten, and W. Sale, "Adhesion of cells to surfaces coated with polylysine. Applications to electron microscopy," *The Journal of Cell Biology*, vol. 66, no. 1, pp. 198–200, 1975.

[10] T. G. Park, J. H. Jeong, and S. W. Kim, "Current status of polymeric gene delivery systems," *Advanced Drug Delivery Reviews*, vol. 58, no. 4, pp. 467–486, 2006.

[11] Z. Kadlecova, Y. Rajendra, M. Matasci et al., "DNA delivery with hyperbranched polylysine: a comparative study with

linear and dendritic polylysine," *Journal of Controlled Release*, vol. 169, no. 3, pp. 276–288, 2013.

[12] Y. Jiang, A. M. Brynskikh, D. S-Manickam, and A. V. Kabanov, "SOD1 nanozyme salvages ischemic brain by locally protecting cerebral vasculature," *Journal of Controlled Release*, vol. 213, pp. 36–44, 2015.

[13] S. Hayat, S. Khan, A. Khan, and J.-B. Liu, "Valency-based molecular descriptors for measuring the π-electronic energy of lower polycyclic aromatic hydrocarbons," *Polycyclic Aromatic Compounds*, vol. 42, no. 4, pp. 1113–1129, 2022.

[14] M. Y. H. Malik, M. Ahsan Binyamin, and S. Hayat, "Correlation ability of degree-based topological indices for physicochemical properties of polycyclic aromatic hydrocarbons with applications," *Polycyclic Aromatic Compounds*, vol. 42, pp. 1–15, 2021.

[15] S. Hayat, S. Khan, M. Imran, and J.-B. Liu, "Quality testing of distance-based molecular descriptors for benzenoid hydrocarbons," *Journal of Molecular Structure*, vol. 1222, Article ID 128927, 2020.

[16] S. Hayat, S. Khan, A. Khan, and M. Imran, "Distance-based topological descriptors for measuring the π-electronic energy of benzenoid hydrocarbons with applications to carbon nanotubes," *Mathematical Methods in the Applied Sciences*, 2020.

[17] S. Hayat, S. Khan, A. Khan, and M. Imran, "A computer-based method to determine predictive potential of distance-spectral descriptors for measuring the- electronic energy of benzenoid hydrocarbons with applications," *IEEE Access*, vol. 9, pp. 19238–19253, 2021.

[18] S. Hayat and S. Khan, "Quality testing of spectrum-based valency descriptors for polycyclic aromatic hydrocarbons with applications," *Journal of Molecular Structure*, vol. 1228, no. 2021, Article ID 129789, 2021.

[19] M. Y. H. Malik, S. Hayat, S. Khan, and M. A. Binyamin, "Predictive potential of spectrum-based topological descriptors for measuring theπ-electronic energy of benzenoid hydrocarbons with applications to boron triangular and boronα-nanotubes," *Mathematical Methods in the Applied Sciences*, 2021.

[20] A. Doley, J. Buragohain, and A. Bharali, "Inverse sum indeg status index of graphs and its applications to octane isomers and benzenoid hydrocarbons," *Chemometrics and Intelligent Laboratory Systems*, vol. 203, Article ID 104059, 2020.

[21] S. Mondal, N. De, and A. Pal, "On some general neighborhood degree based topological indices," *International Journal of Apllied Mathematics*, vol. 32, no. 6, p. 1037, 2020.

[22] M. C. Shanmukha, N. S. Basavarajappa, A. Usha, and K. C. Shilpa, "Novel neighbourhood redefined first and second Zagreb indices on carborundum structures," *Journal of Applied Mathematics and Computing*, vol. 66, no. 1-2, pp. 263–276, 2021.

[23] A. Usha, M. C. Shanmukha, K. C. Shilpa, and B. M. Praveen, "Comparative study of degree-based molecular descriptors of cyclodextrins through M-polynomial and NM-polynomial," *Journal of the Indian Chemical Society*, vol. 100, no. 6, Article ID 100999, 2023.

[24] M. C. Shanmukha, S. Lee, A. Usha, K. C. Shilpa, and M. Azeem, "Structural descriptors of anthracene using topological coindices through CoM-polynomial," *Journal of Intelligent and Fuzzy Systems*, vol. 44, pp. 1–12, 2023.

[25] M. C. Shanmukha, A. Usha, K. C. Shilpa, and M. K. Siddiqui, "Structural investigation of carbon nanocone through topological coindices," *International Journal of Quantum Chemistry*, vol. 123, no. 12, Article ID e27109, 2023.

[26] H. Hosoya, "On some counting polynomials in chemistry," *Discrete Applied Mathematics*, vol. 19, no. 1–3, pp. 239–257, 1988.

[27] E. Deutsch and S. Klav zar, "M-Polynomial and degree-based topological indices," *Iranian Journal of Mathematical Chemistry*, vol. 6, no. 2, pp. 93–102, 2015.

[28] S. Mondal, N. De, A. Pal, and A. Pal, "Topological properties of Graphene using some novel neighborhood degree-based topological indices," *International Journal of Mathematics for Industry*, vol. 11, no. 01, pp. 9915–9927, 2020.

[29] H. Mohammed Yasin, M. Suresh, G. A. Abebe, and S. A. Fufa, "Results on certain biopolymers using M-polynomial and NM-polynomial of topological indices," *Computational and Mathematical Methods in Medicine*, vol. 2023, Article ID 4668505, 15 pages, 2023.

[30] M. Munir, W. Nazeer, S. Rafique, and S. M. Kang, "M-polynomial and degree-based topological indices of polyhex nanotubes," *Symmetry*, vol. 8, no. 12, p. 149, 2016.

[31] A. Ali, W. Nazeer, M. Munir, and S. Min Kang, "M-polynomials and topological indices of zigzag and rhombic benzenoid systems," *Open Chemistry*, vol. 16, no. 1, pp. 73–78, 2018.

[32] M. Munir, W. Nazeer, A. R. Nizami, S. Rafique, and S. M. Kang, "M-polynomials and topological indices of titania nanotubes," *Symmetry*, vol. 8, no. 11, p. 117, 2016.

[33] S. Mondal, M. Imran, N. De, and A. Pal, "Neighborhood M-polynomial of titanium compounds," *Arabian Journal of Chemistry*, vol. 14, no. 8, Article ID 103244, 2021.

[34] X. Zuo, M. Numan, S. I. Butt, M. K. Siddiqui, R. Ullah, and U. Ali, "Computing topological indices for molecules structure of Polyphenylene via M-polynomials," *Polycyclic Aromatic Compounds*, vol. 42, no. 4, pp. 1103–1112, 2022.

[35] H. Mohammed Yasin and M. Suresh, "Results on certain polymers using m-polynomial and nm-polynomial of topological indices," 2022, https://europepmc.org/article/ppr/ppr547889.

[36] M. K. Siddiqui, S. Javed, S. Khalid, N. Amin, and M. Hussain, "On network construction and module detection for molecular graph of titanium dioxide," *Journal of Biomolecular Structure and Dynamics*, vol. 41, no. 20, pp. 10591–10603, 2022.

[37] A. Ullah, A. Zeb, and S. Zaman, "A new perspective on the modeling and topological characterization of H-Naphtalenic nanosheets with applications," *Journal of Molecular Modeling*, vol. 28, no. 8, p. 211, 2022.

[38] K. Bhubalan, J. A. Chuah, F. Shozui et al., "Characterization of the highly active polyhydroxyalkanoate synthase of Chromobacterium sp. strain USM2," *Applied and Environmental Microbiology*, vol. 77, no. 9, pp. 2926–2933, 2011.

[39] C. F. Budde, S. L. Riedel, F. Hübner et al., "Growth and polyhydroxybutyrate production by Ralstonia eutropha in emulsified plant oil medium," *Applied Microbiology and Biotechnology*, vol. 89, no. 5, pp. 1611–1619, 2011.

[40] K. Sudesh, H. Abe, and Y. Doi, "Synthesis, structure and properties of polyhydroxyalkanoates: biological polyesters," *Progress in Polymer Science*, vol. 25, no. 10, pp. 1503–1555, 2000.

[41] M. Imran, M. Naeem, and A. Q. Baig, "Topological indices of polyhydroxybutyrate and polycaprolactone," *Journal of Information and Optimization Sciences*, vol. 41, no. 4, pp. 1025–1041, 2020.