Elucidating structure–property relationships of guar gum biomolecules: insights from $\mathbb{M}$-polynomial and QSPR modeling

Waheed Khalid and Shamaila Yousaf*

Department of Mathematics, University of Gujrat, Gujrat, Pakistan

This study investigates the quantitative structure–property relationship (QSPR) modeling of guar gum biomolecules, focusing on their structural parameters. Guar gum, a polysaccharide with diverse industrial applications, exhibits various properties such as viscosity, solubility, and emulsifying ability, which are influenced by its molecular structure. In this research, $\mathbb{M}$-polynomial and associated topological indices are employed as structural descriptors to represent the molecular structure of guar gum. The $\mathbb{M}$-polynomial and associated topological indices capture important structural features, including size, shape, branching, and connectivity. By correlating these descriptors with experimental data on guar gum properties, predictive models are developed using regression analysis techniques. The analysis revealed a strong correlation between the boiling point and molecular weight and all the considered topological descriptors. The resulting models offer insights into the relationship between guar gum structure and its properties, facilitating the optimization of guar gum production and application in various industries. This study demonstrates the utility of $\mathbb{M}$-polynomial and QSPR modeling in elucidating structure–property relationships of complex biomolecules like guar gum, contributing to the advancement of biomaterial science and industrial applications.

KEYWORDS

chemical graph theory, QSPR, physicochemical properties, M-polynomials, topological indices, guar gum

1 Introduction

Guar gum, an innovative agrochemical, is derived from the endosperm of cluster beans. The species *Cyamopsis tetragonoloba*, belonging to the Leguminosae family, produces the seeds used in guar gum production, and these seeds are resistant to drought (Prem et al., 2005). The concept of transdomestication was introduced by Hymowitz, although the exact origins of this practice are still a matter of dispute. Further information on the subject can be found in Whistler (1948) and BeMiller (2009). Guar gum has recently piqued the curiosity of several experts for numerous reasons. Guar gum powder serves as a thickener, stabilizer, and health management tool in various industries. It consists of galactomannan polysaccharides and can be derived from different sources, including algae, plants, microorganisms, and animals (Hovgaard and Brondsted, 1996). These polysaccharides

are characterized by their stability, non-toxicity, hydrophilicity, and biodegradability. Its unique properties, such as high viscosity, solubility, and stability, make it a versatile ingredient with a wide range of applications in industries like food, pharmaceuticals, cosmetics, and oil drilling. Additionally, guar gum is known for its biocompatibility and non-toxic nature, making it suitable for various biomedical and pharmaceutical applications. By studying guar gum, researchers can explore its potential uses, optimize its properties, and develop innovative products with improved performance and functionality. Overall, the selection of guar gum for research offers opportunities to advance knowledge in various fields and contribute to the development of sustainable and high-performing materials and products.

Various derivatives of guar gum exist, such as carboxymethyl guar $\mathcal{HPG}$, hydroxymethyl guar $\mathcal{CMG}$, hydroxypropylethyl guar, ammonium hydroxylpropyl trimethyl chloride guar, acryloyloxy guar, methacryloyl guar, guar gum esters, and carboxymethyl hydroxypropyl guar $\mathcal{CMHPG}$. The computation of guar gum and its derivatives employs molecular graphs, as detailed in Shanmukha et al. (2022). The most widely used derivatives are carboxymethyl guar ($\mathcal{CMG}$), hydroxypropyl guar ($\mathcal{HPG}$), and carboxymethyl hydroxypropyl guar ($\mathcal{CMHPG}$), which are discussed in this study with respect to topological indices.

Chemical graph theory is an interdisciplinary field that links chemistry and mathematics. Graph modeling, originating from early chemical experiments, is a crucial aspect of theoretical chemistry. The subfield of cheminformatics analyzes quantitative structure–activity relationships ($\mathcal{QSAR}$) and quantitative structure–property relationships ($\mathcal{QSPR}$) to predict the biological activity and characteristics of guar gum and its derivatives. Utilizing topological indices and physico-chemical substances, it is possible to infer the pharmacological activity of these compounds without conducting experiments. Noteworthy, studies related to topological indices and physico-chemical substances include Arockiaraj et al. (2023a); Arockiaraj et al. (2023b); and Arockiaraj et al. (2023c). Recently, algebraic polynomials, such as the Hosoya polynomial (Consonni and Todeschini, 2010a) and M-polynomials (Deutsch and Klavar, 2014), have gained prominence in chemistry for determining distance-based topological indices and degree-based topological indices, respectively. The M-polynomial yields closed forms for various degree-based indices, while the Hosoya polynomial focuses on distance-based indices. The M-polynomial, often denoted as $\mathbb{M}(x, y)$, is a polynomial used in the study of chemical graph theory, particularly in the enumeration of certain chemical structures known as molecular graphs. The M-polynomial encodes information about the molecular graph's topology, such as its number of vertices, edges, and other structural properties. It has applications in the enumeration of molecular isomers, the prediction of molecular properties, and the study of chemical reactions. Significant knowledge regarding degree-based graph invariants can be found in the M-polynomial literature, including Munir et al. (2016a); Munir et al. (2016b); Munir et al. (2016c); Munir et al. (2016d); and Ajmal et al. (2017). There is a wealth of knowledge regarding degree-based graph invariants in the M-polynomial.

TABLE 1 M-polynomials are used to derive several degree-based topological indices.

$TopologicalIndex$	$Derivation from \mathbb{M}(\Gamma; x, y)$
M_1	$(\mathcal{D}_x + \mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
M_2	$(\mathcal{D}_x \mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
$^m M_2$	$(\mathcal{S}_x \mathcal{S}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
R_α	$(\mathcal{D}_x^\alpha \mathcal{D}_y^\alpha)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
RR_α	$(\mathcal{S}_x^\alpha \mathcal{S}_y^\alpha)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
SDD	$(\mathcal{D}_x \mathcal{S}_y + \mathcal{S}_x \mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
H	$2(\mathcal{S}_x \mathcal{I})(\mathbb{M}(\Gamma; x, y))|_{x=1}$
I	$(\mathcal{S}_x \mathcal{I} \mathcal{D}_x \mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=1}$
AZI	$(\mathcal{S}_x^3 \mathcal{Q}_{-2} \mathcal{I} \mathcal{D}_x^3 \mathcal{D}_y^3)(\mathbb{M}(\Gamma; x, y))|_{x=1}$

The M-polynomial of graph Γ is defined as

$$\mathbb{M}(\Gamma; x, y) = \sum_{s \leq t} m_{st}(\Gamma) x^s y^t,$$

where $m_{st}(\Gamma)$ is the number of edges $vv \in E(\Gamma)$ such that $\{d_v, d_v\} = \{s, t\}$.

Table 1 contains some degree-based TIs and the M-polynomial for the graph Γ: $\mathcal{D}_x = x \frac{\partial(g(x,y))}{\partial(x)}$, $\mathcal{D}_y = y \frac{\partial(g(x,y))}{\partial(y)}$, $\mathcal{S}_x = \int_0^x \frac{g(t,y)}{t} dt$, $\mathcal{S}_y = \int_0^y \frac{g(x,t)}{t} dt$, $\mathcal{I}(g(x, y)) = (g(x, x))$, and $\mathcal{Q}_\alpha(g(x, y)) = x^\alpha(g(x, y))$.

The topological index, frequently known as the connectedness index, was introduced in 1947 as a result of Weiner's research (Consonni and Todeschini, 2010b). The earliest and most extensively researched topological index was the Wiener index [for further information, see (Wiener, 1947; Gutman et al., 1986)]. One of the earliest topological indices, the Randić index (Randic, 1975), was first introduced by Milan Randić in 1975 and is represented by the symbol $R_{-\frac{1}{2}}(\Gamma)$. Its definition is as follows:

$$R_{-\frac{1}{2}}(\Gamma) = \sum_{vv \in E(\Gamma)} \frac{1}{\sqrt{d_v d_v}}. \qquad (1)$$

In 1998, Bollobs and Erds (1998) and Amic et al. (1998) independently proposed the general Randić index, which has been extensively studied for its numerous mathematical properties (Caporossi et al., 2003; Hu et al., 2005). For a detailed survey, refer to Li et al. (2006). The general Randić index is defined as

$$R_\alpha(\Gamma) = \sum_{vv \in E(\Gamma)} \frac{1}{(d_v d_v)^\alpha}, \qquad (2)$$

and $RR_\alpha(\Gamma) = \sum_{vv \in E(\Gamma)} (d_v d_v)^\alpha$ is the definition of the inverse Randić index.

Many papers and books, such as Kier and Hall (1976) and Kier and Hall (1986), have been produced on this topological index. For drug design, the Randić index was recognized. The first and second Zagreb indices were introduced by Gutman and Trinajstić. They are denoted as follows: $M_1(\Gamma) = \sum_{vv \in E(\Gamma)}(d_v + d_v)$ and $M_2(\Gamma) = \sum_{vv \in E(\Gamma)}(d_v d_v)$, respectively. The reader is referred to Nikolic et al. (2003); Das and Gutman (2004); Gutman and Das (2004); Vukicevic and Graovac (2004); and Trinajstic et al. (2010) for

FIGURE 1
Molecular structure. **(A)** guar gum, **(B)** HPG, **(C)** CMG, and **(D)** CMHPG.
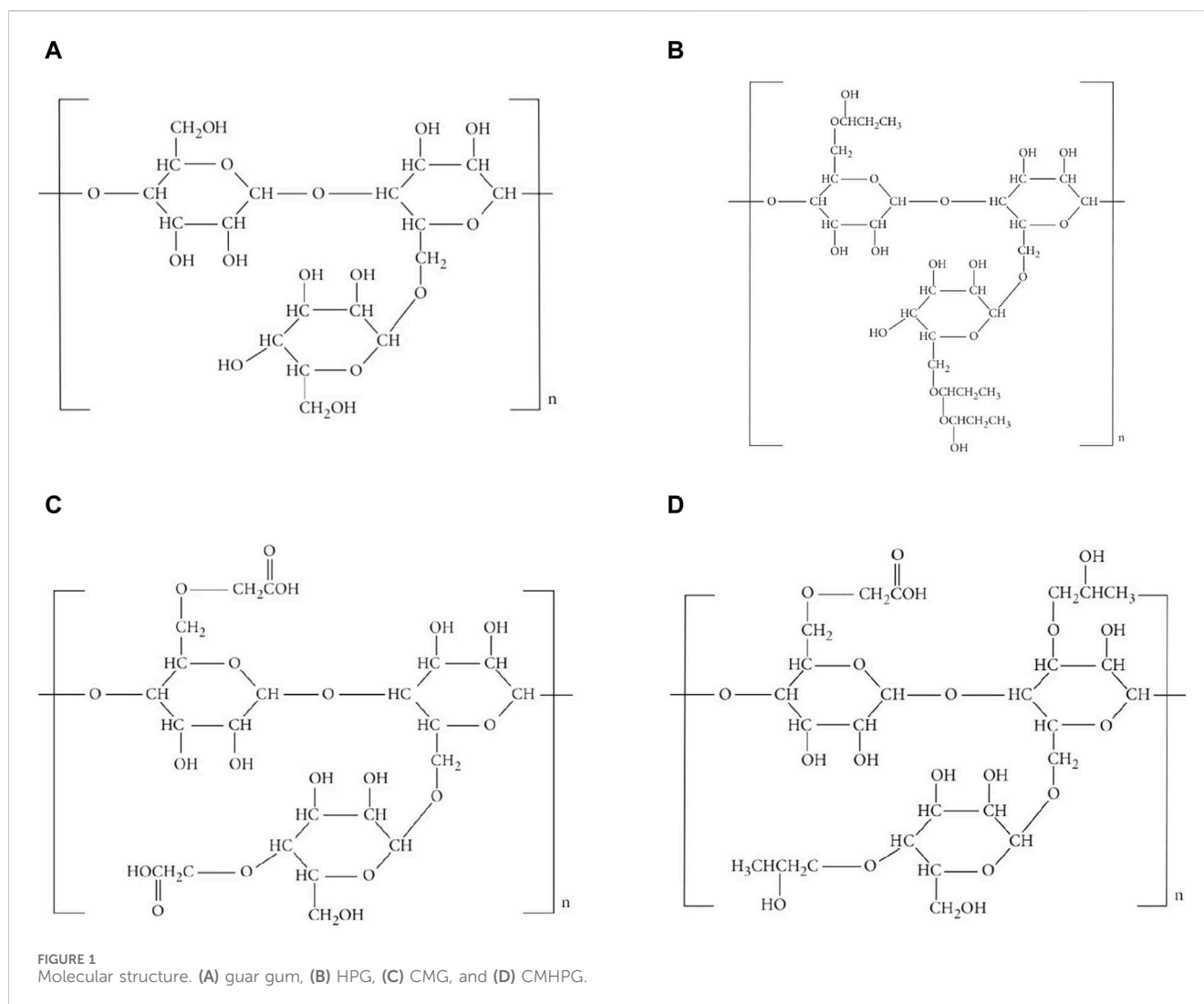
further information on these indices. Among several modifications of Zagreb indices, one is the second modified Zagreb index. According to Milicevic et al. (2004), the second modified Zagreb index for a simple connected graph Γ is defined as

$$^{m}M_{2}(\Gamma) = \sum_{\upsilon\nu\in E(\Gamma)} \frac{1}{d_{\upsilon}d_{\nu}} \qquad (3)$$

The symmetric division index (SDD) is particularly useful in determining the total surface area for polychlorobiphenyls (Gupta et al., 2016) based on the discrete Adriatic indices. The symmetric division index of a connected graph G is defined as

$$SDD(\Gamma) = \sum_{\upsilon\nu\in E(\Gamma)} \left\{ \frac{\min(d_{\upsilon},d_{\nu})}{\max(d_{\upsilon},d_{\nu})} + \frac{\max(d_{\upsilon},d_{\nu})}{\min(d_{\upsilon},d_{\nu})} \right\}. \qquad (4)$$

The harmonic index is an additional Randić index variation that is described as

$$H(\Gamma) = \sum_{\upsilon\nu\in E(\Gamma)} \frac{2}{d_{\upsilon}+d_{\nu}}. \qquad (5)$$

There is a relationship between graph eigenvalues and the harmonic index (Favaron et al., 1993). Using MathChem, the elegant structure of extremal graphs is used to generate the inverse sum index (Balaban, 1982), a significant predictor of the octane isomer total surface area.

$$I(\Gamma) = \sum_{\upsilon\nu\in E(\Gamma)} \frac{d_{\upsilon}d_{\nu}}{d_{\upsilon}+d_{\nu}}. \qquad (6)$$

Furtula et al. (2010) is credited for the augmented Zagreb index AZI, which is characterized as

$$AZI(\Gamma) = \sum_{\upsilon\nu\in E(\Gamma)} \left\{ \frac{d_{\upsilon}d_{\nu}}{d_{\upsilon}+d_{\nu}-2} \right\}^{3}. \qquad (7)$$

Graph invariant AZI has higher prediction power than the atom-bond connectivity index (Furtula et al., 2010) and is a useful predictive measure for analyzing the heat of formation in octanes and heptanes (for more detail, see (Estrada et al., 1998; Das, 2010)). A few well-known degree-based topological indices (which are defined in Eqs 1–7) with $\mathbb{M}$-polynomials (Deutsch and Klavar, 2014) are related in the following Table 1.

FIGURE 2
Comparison of topological indices of guar gum in blue, $\mathcal{HPG}$ and $\mathcal{CMG}$ in yellow, and $\mathcal{CMHPG}$ in green, respectively. **(A)** M_1, **(B)** M_2, **(C)** $^mM_2$, **(D)** SDD, **(E)** H, **(F)** I, and **(G)** AZI.
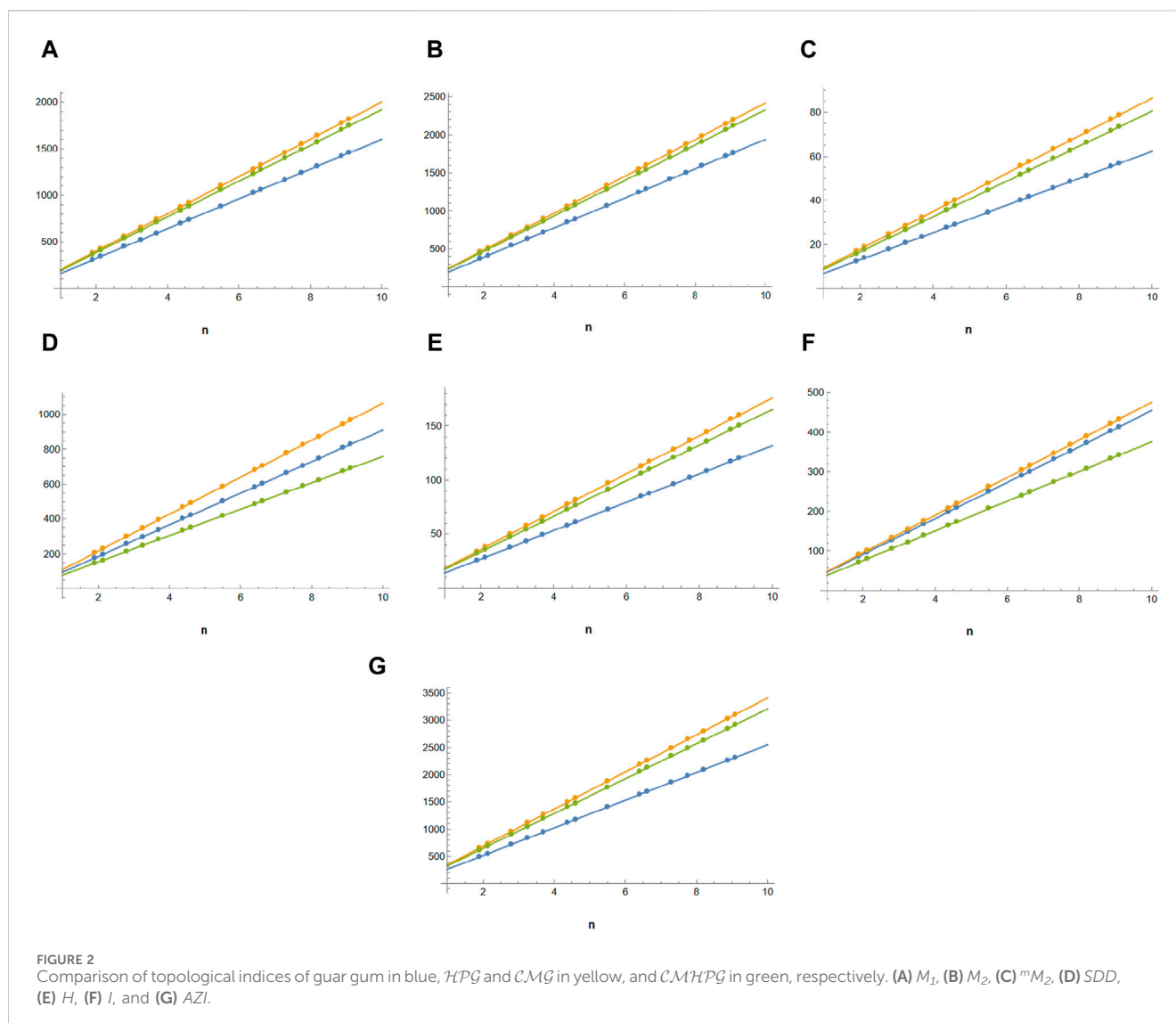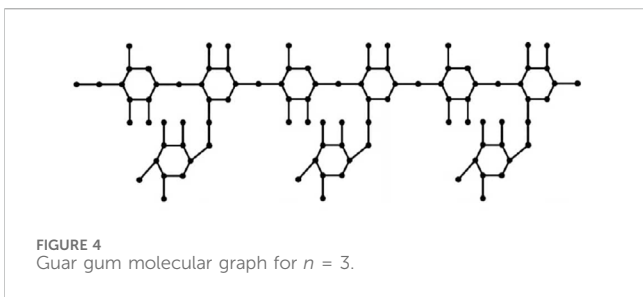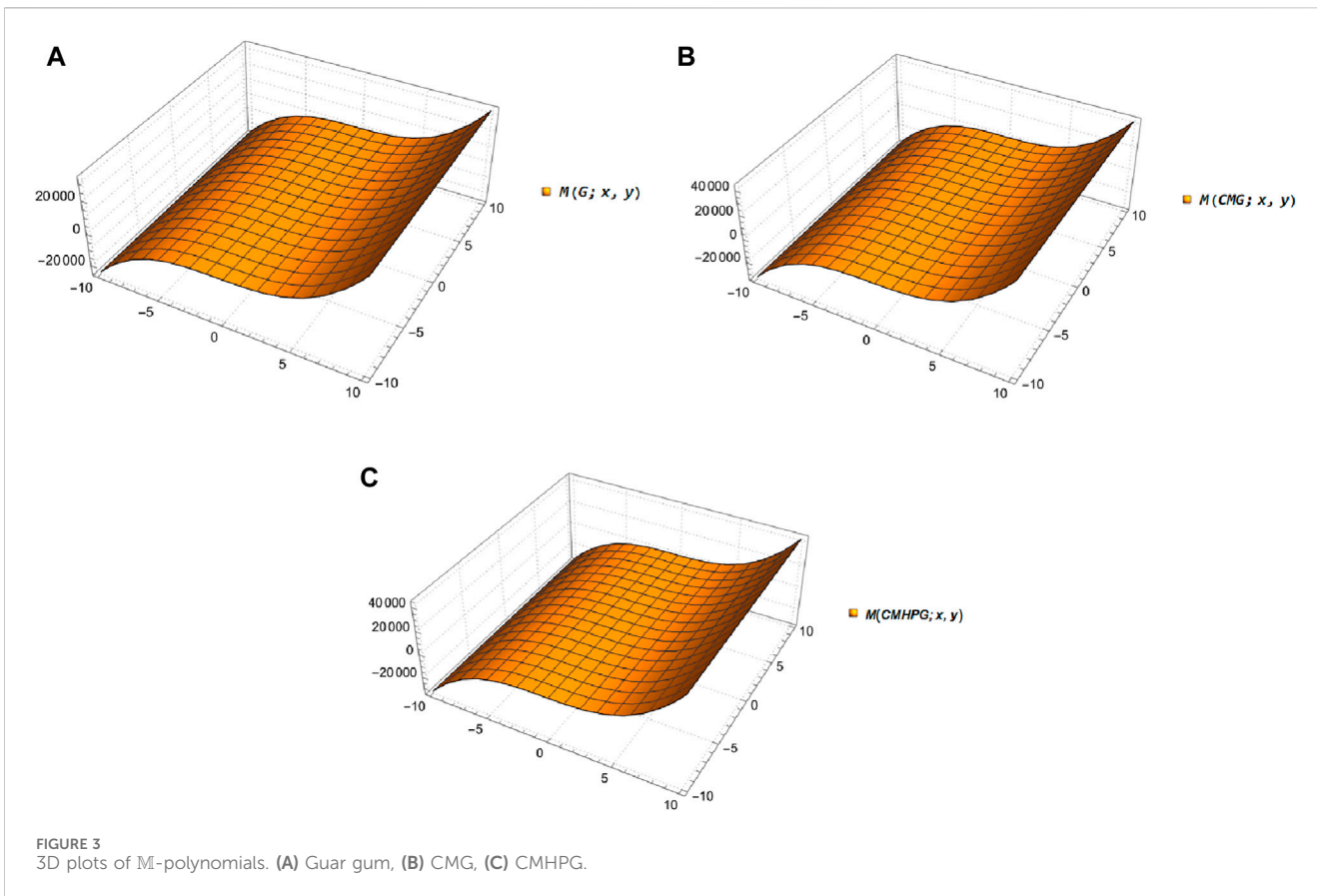
2 Methodology

Molecular graphs and vertex and edge partitions are used to modify the molecular structure of guar gum and its chemical derivatives (Figure 1). Topological indices are derived using $\mathbb{M}$-polynomial. Graphical comparisons of the aforementioned defined indices are made using vertex partition, edge partition, and combinatorial computing. The graphical representation of the outcomes and the comparative study of the findings are performed via 2D plotting in Figure 2 and 3D plotting in Figure 3 are shown by utilizing Mathematica software. In this study, physio-chemical properties of the selected guar gum and its derivatives were obtained from ChemSpider, providing a comprehensive dataset for analysis. Several topological indices were calculated using $\mathbb{M}$-polynomials, extracting key molecular information relevant to biological activities. Subsequently, these indices were utilized in quantitative structure–property relationship (QSPR) analysis, employing SPSS software. The process involves constructing linear, quadratic, and logarithmic models to establish correlations between the calculated topological indices and the properties of selected guar gum and its derivatives. This meticulous methodology aims to uncover patterns and relationships within the molecular structures, contributing to a deeper understanding of the properties of selected guar gum and its derivatives.

3 Main results and discussions

This section outlines our primary analytical findings and subdivides the material into three sections: guar gum, hydroxypropyl guar, and carboxymethyl guar. The $\mathbb{M}$-polynomials and their associated topological indices are derived for the chemical structures of guar gum, which are useful in the QSPR study. Guar gum is a polysaccharide used in various industries including food, pharmaceuticals, and cosmetics. QSPR studies based on $\mathbb{M}$-polynomials and topological indices can help in understanding how its structural features relate to its properties such as viscosity, solubility, and emulsifying ability. By establishing quantitative relationships between structure and properties, researchers can optimize the production and application of guar gum for various industrial purposes.

FIGURE 3
3D plots of $\mathbb{M}$-polynomials. **(A)** Guar gum, **(B)** CMG, **(C)** CMHPG.

FIGURE 4
Guar gum molecular graph for $n = 3$.

3.1 Guar gum

This section uses various topological indices to analyze the molecular graph of guar gum. Figure 4 shows the vertex and edge partitioning of guar gum.

$$E_{\{i_0,i_1\}} = \{e = vv \in E(\Gamma[m,n]): d_v = i_0, d_v = i_1\},$$

such that $|E_{\{1,2\}}| = 1$, $|E_{\{1,3\}}| = 7n + 1$, $|E_{\{2,2\}}| = 2n$, $|E_{\{2,3\}}| = 14n - 1$, and $|E_{\{3,3\}}| = 9n$.

Theorem 3.2: *Consider a molecular graph Γ for guar gum. Then,*

$$\mathbb{M}(\Gamma; x, y) = xy^2 + (7n + 1)xy^3 + 2nx^2y^2 + (14n - 1)x^2y^3 + 9nx^3y^3.$$

Proof. Using the $\mathbb{M}$-polynomial of Γ, we obtain the following equation:

$$\mathbb{M}(\Gamma; x, y) = \sum_{i_0 \le i_1} m_{i_0 i_1}(\Gamma)x^{i_0}y^{i_1}.$$

$$= \sum_{1 \le 2} m_{12}(\Gamma)x^1y^2 + \sum_{1 \le 3} m_{13}(\Gamma)x^1y^3 + \sum_{2 \le 2} m_{22}(\Gamma)x^2y^2$$

$$+ \sum_{2 \le 3} m_{22}(\Gamma)x^2y^3 + \sum_{3 \le 3} m_{33}(\Gamma)x^3y^3.$$

$$= \sum_{uv \in E_{\{1,2\}}} m_{12}(\Gamma)x^1y^2 + \sum_{uv \in E_{\{1,3\}}} m_{13}(\Gamma)x^1y^3$$

$$+ \sum_{uv \in E_{\{2,2\}}} m_{22}(\Gamma)x^2y^2 + \sum_{uv \in E_{\{2,3\}}} m_{23}(\Gamma)x^2y^3$$

$$+ \sum_{uv \in E_{\{3,3\}}} m_{33}(\Gamma)x^3y^3.$$

$$= |E_{\{1,2\}}|x^1y^2 + |E_{\{1,3\}}|x^1y^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3$$

$$+ |E_{\{3,3\}}|x^3y^3.$$

$$= xy^2 + (7n + 1)xy^3 + 2nx^2y^2 + (14n - 1)x^2y^3$$

$$+ 9nx^3y^3.$$

Proposition 3.3: *Consider a molecular graph Γ for guar gum. Then,*

1. $M_1(\Gamma) = 160n + 2.$
2. $M_2(\Gamma) = 194n - 1.$
3. $^mM_2(\Gamma) = 6.167n + 0.67.$
4. $R_\alpha(\Gamma) = 2^\alpha + 3^\alpha(7n + 1) + 2^{2\alpha+1}n + 2^\alpha 3^\alpha(14n - 1) + 3^{2\alpha+2}n.$
5. $RR_\alpha(\Gamma) = \dfrac{1}{2^\alpha} + \dfrac{(7n + 1)}{3^\alpha} + \dfrac{n}{2^{2\alpha-1}} + \dfrac{(14n - 1)}{2^\alpha 3^\alpha} + \dfrac{n}{3^{2\alpha-2}}.$
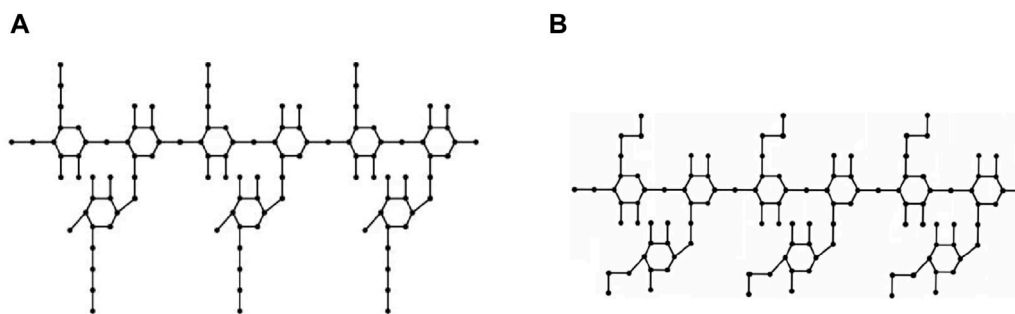6. $SDD(\Gamma) = 75.67n + 2.5.$

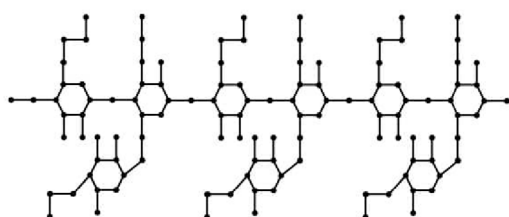FIGURE 5
Molecular graph for n = 3: **(A)** HPG and **(B)** CMG.

FIGURE 6
Molecular graph of $\mathcal{CMHPG}$ for n = 3.

Proof: From the edge partitioning of guar gum and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equations (Eqs 8–16):

$$g(x, y) = \mathbb{M}(\Gamma; x, y)$$
$$= xy^2 + (7n+1)xy^3 + 2nx^2y^2$$
$$+ (14n-1)x^2y^3 + 9nx^3y^3,$$

$$\mathcal{D}_x(g(x, y)) = xy^2 + (7n+1)xy^3 + 4nx^2y^2 + 2(14n-1)x^2y^3$$
$$+ 27nx^3y^3, \qquad (8)$$

$$\mathcal{D}_y(g(x, y)) = xy^2 + 3(7n+1)xy^3 + 4nx^2y^2 + 3(14n-1)x^2y^3$$
$$+ 27nx^3y^3, \qquad (9)$$

$$\mathcal{D}_x\mathcal{D}_y(g(x, y)) = xy^2 + 3(7n+1)xy^3 + 8nx^2y^2 + 6(14n-1)x^2y^3$$
$$+ 81nx^3y^3, \qquad (10)$$

$$\mathcal{S}_x(g(x, y)) = xy^2 + (7n+1)xy^3 + nx^2y^2 + \frac{1}{2}(14n-1)x^2y^3$$
$$+ \frac{9}{3}nx^3y^3, \qquad (11)$$

$$\mathcal{S}_y\mathcal{S}_x(g(x, y)) = \frac{1}{2}xy^2 + \frac{1}{3}(7n+1)xy^3 + \frac{1}{2}nx^2y^2$$
$$+ \frac{1}{6}(14n-1)x^2y^3 + \frac{9}{9}nx^3y^3, \qquad (12)$$

$$\mathcal{D}_x^\alpha\mathcal{D}_y^\alpha(g(x, y)) = 2^\alpha xy^2 + 3^\alpha(7n+1)xy^3 + 2.2^\alpha.2^\alpha nx^2y^2$$
$$+ 2^\alpha.3^\alpha(14n-1)x^2y^3, \qquad (13)$$

$$+ 9n3^\alpha.3^\alpha x^3y^3, \qquad (14)$$

$$\mathcal{S}_y^\alpha\mathcal{S}_x^\alpha(g(x, y)) = \frac{xy^2}{2^\alpha} + \frac{7n+1}{3^\alpha}xy^3 + \frac{nx^2y^2}{2^{\alpha-1}.2^\alpha} + \frac{14n-1}{2^\alpha.3^\alpha}x^2y^3$$
$$+ \frac{9nx^3y^3}{3^\alpha.3^\alpha}, \qquad (15)$$

$$\mathcal{S}_y\mathcal{D}_x(g(x, y)) = \frac{xy^2}{2} + \frac{7n+1}{3}xy^3 + 2nx^2y^2 + \frac{2}{3}(14n-1)x^2y^3$$
$$+ 9nx^3y^3, \qquad (16)$$

$$\mathcal{S}_x\mathcal{D}_y(g(x, y)) = 2xy^2 + 3(7n+1)xy^3 + 2nx^2y^2$$
$$+ \frac{3}{2}(14n-1)x^2y^3 + 9nx^3y^3. \qquad (17)$$

From Table 1, we obtain the following equation:

1. $M_1(\Gamma) = (\mathcal{D}_x + \mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1} = 160n + 2.$
2. $M_2(\Gamma) = (\mathcal{D}_x\mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1} = 194n - 1.$
3. $^mM_2(\Gamma) = (\mathcal{S}_x\mathcal{S}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1} = 6.167n + 0.67.$
4. $R_\alpha(\Gamma) = (\mathcal{D}_x^\alpha\mathcal{D}_y^\alpha)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
$$= 2^\alpha + 3^\alpha(7n+1) + 2^{2\alpha+1}n + 2^\alpha 3^\alpha(14n-1) \quad + 3^{2\alpha+2}n.$$
5. $RR_\alpha(\Gamma) = (\mathcal{S}_x^\alpha\mathcal{S}_y^\alpha)(\mathbb{M}(\Gamma; x, y))|_{x=y=1}$
$$= \frac{1}{2^\alpha} + \frac{(7n+1)}{3^\alpha} + \frac{n}{2^{2\alpha-1}} + \frac{(14n-1)}{2^\alpha 3^\alpha} + \frac{n}{3^{2\alpha-2}}.$$
6. $SDD(\Gamma) = (\mathcal{D}_x\mathcal{S}_y + \mathcal{S}_x\mathcal{D}_y)(\mathbb{M}(\Gamma; x, y))|_{x=y=1} = 75.67n + 2.5.$

Proposition 3.4: *Consider a molecular graph Γ for guar gum. Then,*

1. $H(\Gamma) = 13.1n + 0.76.$
2. $I(\Gamma) = 37.55n + 0.22.$
3. $AZI(\Gamma) = 254.125n + 3.375.$

Proof: From the edge partitioning of guar gum and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equations (Eqs 17–20):

$$g(x, y) = \mathbb{M}(\Gamma; x, y)$$
$$= xy^2 + (7n+1)xy^3 + 2nx^2y^2 + (14n-1)x^2y^3 + 9nx^3y^3.$$

FIGURE 7
Molecular structures of carbohydrates: **(A)** arabinose, **(B)** galactose, **(C)** maltose, **(D)** sucrose, **(E)** sorbose, **(F)** ribose, **(G)** hydroxymethyl furfural (HMF), and **(H)** raffinose.
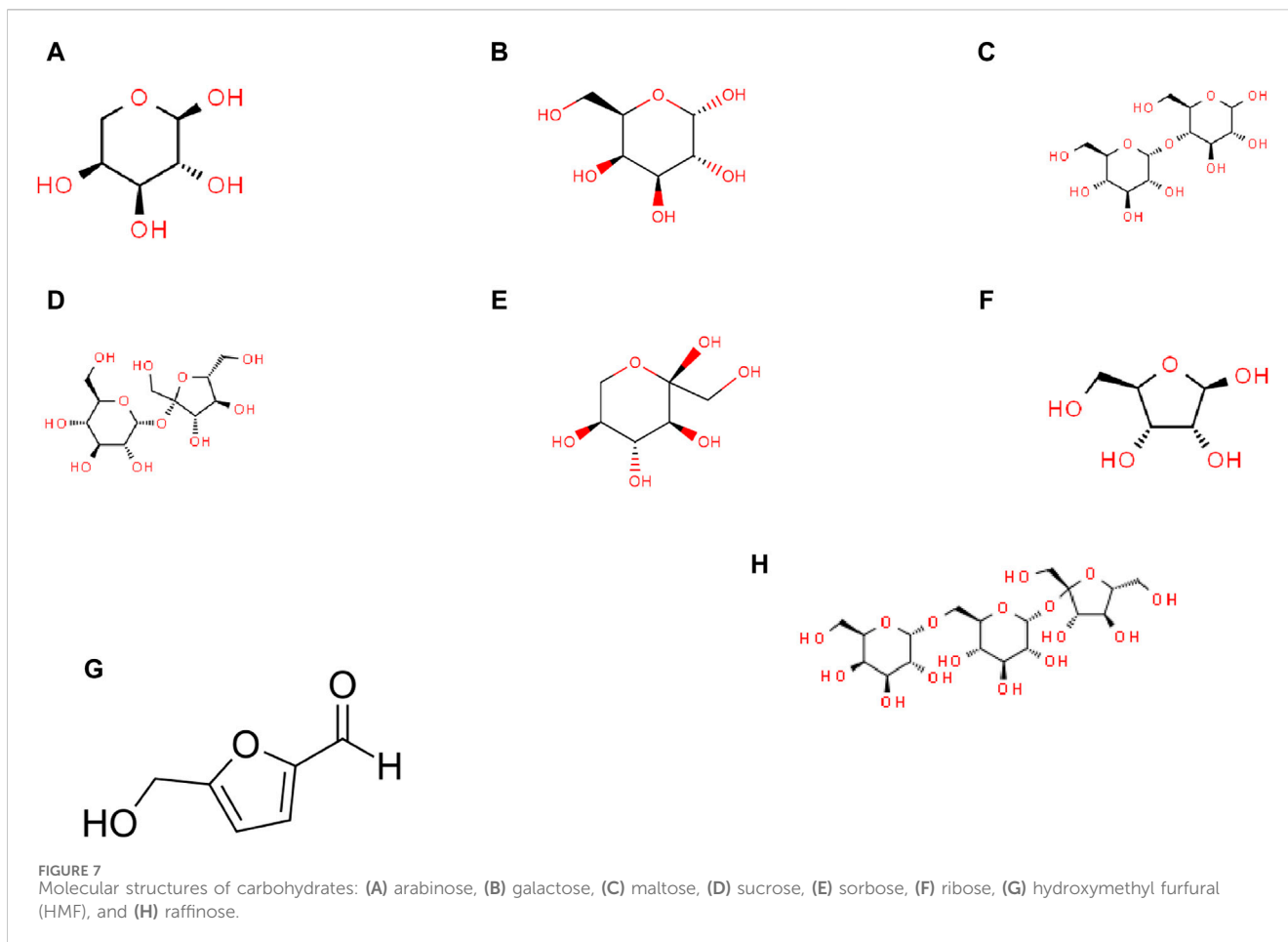
TABLE 2 Properties of aforementioned structures.

Structure	Density	Boiling Point (BP)	Melting Point (MP)	Molecular Weight (MW)	Water Solubility (WS)
Unit	g/cm³	°C	°C	g/mol	g/L
Arabinose	1.585	415.5	164	150.13	834
Galactose	1.5	232.96	168	180.156	650
Maltose	1.54	397.76	160	342.297	310
Sucrose	1.587	697.1	186	342.30	200
Sorbose	1.65	551.7	165	180	550
Ribose	1.5	415.5	95	150.13	100
HMP	1.29	114	30	126.11	83
Raffinose	884.8	363.0	81	504.44	229.8

$$\mathcal{I}\left(g\left(x,y\right)\right) = x^3 + (7n+1)x^4 + 2nx^4 + 2\left(14n-1\right)x^5 + 9nx^6, \quad (18)$$

$$\mathcal{S}_x\mathcal{I}\left(g\left(x,y\right)\right) = \frac{1}{3}x^3 + \frac{(7n+1)}{4}x^4 + \frac{1}{2}nx^4 + \frac{1}{5}\left(14n-1\right)x^5 + \frac{3}{2}nx^6, \quad (19)$$

$$\mathcal{S}_x\mathcal{I}\mathcal{D}_x\mathcal{D}_y\left(g\left(x,y\right)\right) = \frac{2}{3}x^3 + \frac{3\left(7n+1\right)}{4}x^4 + 2nx^4 + \frac{6}{5}\left(14n-1\right)x^5 + \frac{27}{2}nx^6, \quad (20)$$

TABLE 3 Computation of topological indices.

Structure	H	I	AZI	M_1	M_2	${}^m M_2$	SDD
Arabinose	4.3	10.9	71.6719	48	55	2.25	25.6667
Galactose	5.2	13.2667	91.0625	59	68	2.7778	30.3333
Maltose	10.2	27.4333	191.375	118	143	5.2222	58.3333
Sucrose	10.4333	27.05	192.6094	116	138	5.4444	57.6667
Sorbose	5.0875	12.2976	89.1006	60	71	2.7222	32
Ribose	4.3667	11.0167	66.4375	48	56	2.3333	25
HMP	4.9	10.2	80	46	49	2.25	25
Raffinose	14.3857	39.0143	271.3396	169	205	7.275	83.25

$$\mathcal{S}_x^3 \mathcal{Q}_{-2} \mathcal{ID}_x^3 \mathcal{D}_y^3 (g(x,y)) = 8x + \frac{27(7n+1)}{8}x^2 + 16nx^2$$
$$+ 8(14n-1)x^3 + \frac{9.27.27}{64}nx^4. \quad (21)$$

From Table 1, we obtain the following equation:

1. $H(\Gamma) = 2(\mathcal{S}_x \mathcal{I})(\mathbb{M}(\Gamma;x,y))|_{x=1} = 13.1n + 0.76.$
2. $I(\Gamma) = (\mathcal{S}_x \mathcal{ID}_x \mathcal{D}_y)(\mathbb{M}(\Gamma;x,y))|_{x=1} = 37.55n + 0.22.$
3. $AZI(\Gamma) = (\mathcal{S}_x^3 \mathcal{Q}_{-2}\mathcal{ID}_x^3 \mathcal{D}_y^3)(\mathbb{M}(\Gamma;x,y))|_{x=1} = 254.125n + 3.375.$

3.2 Results of $\mathcal{HPG}$ and $\mathcal{CMG}$ molecular graphs

When the chemical derivatives of guar gum, such as $\mathcal{HPG}$ and $\mathcal{CMG}$, were developed into molecular graphs. The results for these chemical derivatives were combined, as shown below, because the vertex and edge partitions are similar. Figure 5 shows the molecular graphs of $\mathcal{HPG}$ and $\mathcal{CMG}$. From the vertices and edges of $\mathcal{HPG}$ and $\mathcal{CMG}$, we obtain the following equation:

$$E_{\{i_0,i_1\}} = \{e = uv \in E(\mathcal{CMG}[m,n]): d_v = i_0, d_v = i_1\},$$

such that $|E_{\{1,2\}}| = 2n+1$, $|E_{\{1,3\}}| = 7n+1$, $|E_{\{2,2\}}| = 4n$, $|E_{\{2,3\}}| = 14n-1$, and $|E_{\{3,3\}}| = 12n$.

Theorem 3.6: *Consider a molecular graph Γ for hydroxypropyl Guar and carboxymethyl guar. Then,*

$$\mathbb{M}(\mathcal{CMG};x,y) = (2n+1)xy^2 + (7n+1)xy^3 + 4nx^2y^2$$
$$+ (14n-1)x^2y^3 + 12nx^3y^3.$$

Proof: From the edge partitioning of $\mathcal{HPG}$ and $\mathcal{CMG}$ and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equation:

$$\mathbb{M}(\mathcal{CMG};x,y) = \sum_{i_0 \leq i_1} m_{i_0 i_1}(\Gamma)x^{i_0} y^{i_1}.$$
$$= \sum_{1\leq 2} m_{12}(\Gamma)x^1 y^2 + \sum_{1\leq 3} m_{13}(\Gamma)x^1 y^3$$
$$+ \sum_{2\leq 2} m_{22}(\Gamma)x^2 y^2 + \sum_{2\leq 3} m_{22}(\Gamma)x^2 y^3$$
$$+ \sum_{3\leq 3} m_{33}(\Gamma)x^3 y^3.$$
$$= \sum_{uv\in E_{\{1,2\}}} m_{12}(\Gamma)x^1 y^2 + \sum_{uv\in E_{\{1,3\}}} m_{13}(\Gamma)x^1 y^3$$
$$+ \sum_{uv\in E_{\{2,2\}}} m_{22}(\Gamma)x^2 y^2 + \sum_{uv\in E_{\{2,3\}}} m_{23}(\Gamma)x^2 y^3$$
$$+ \sum_{uv\in E_{\{3,3\}}} m_{33}(\Gamma)x^3 y^3.$$
$$= |E_{\{1,2\}}|x^1 y^2 + |E_{\{1,3\}}|x^1 y^3 + |E_{\{2,2\}}|x^2 y^2$$
$$+ |E_{\{2,3\}}|x^2 y^3 + |E_{\{3,3\}}|x^3 y^3.$$
$$= (2n+1)xy^2 + (7n+1)xy^3 + 4nx^2 y^2$$
$$+ (14n-1)x^2 y^3 + 12nx^3 y^3.$$

Proposition 3.7: *Consider a molecular graph Γ for hydroxypropyl guar and carboxymethyl guar. Then,*

1. $M_1(\Gamma) = 192n + 1.$
2. $M_2(\Gamma) = 233n - 1.$
3. ${}^m M_2(\Gamma) = 7.99n + 0.663.$
4. $R_\alpha(\Gamma) = 2^\alpha(2n+1) + 3^\alpha(7n+1) + 2^{2\alpha+2}n + 2^\alpha 3^\alpha(14n-1)$
$$+ 4.3^{2\alpha+1}n.$$
5. $RR_\alpha(\Gamma) = \frac{1}{2^\alpha}(2n+1) + \frac{(7n+1)}{3^\alpha} + \frac{n}{2^{2\alpha-2}} + \frac{(14n-1)}{2^\alpha 3^\alpha} + \frac{4n}{3^{2\alpha-1}}.$
6. $SDD(\Gamma) = 90.66n + 3.66.$

Proof: From the edge partitioning of $\mathcal{HPG}$ and $\mathcal{CMG}$ and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equations (Eqs 21–30):

TABLE 4 Vertex and edge partitioning of arabinose.

(d_v, d_y)	Frequency
(1,3)	4
(2,2)	1
(2,3)	2
(3,3)	3

TABLE 5 Vertex and edge partitioning of galactose.

(d_v, d_y)	Frequency
(1,2)	1
(1,3)	4
(2,3)	3
(3,3)	4

TABLE 6 Vertex and edge partitioning of maltose.

(d_v, d_y)	Frequency
(1,2)	2
(1,3)	6
(2,3)	8
(3,3)	8

TABLE 7 Vertex and edge partitioning of sucrose.

(d_v, d_y)	Frequency
(1,2)	3
(1,3)	5
(2,3)	9
(3,3)	7

TABLE 8 Vertex and edge partitioning of sorbose.

(d_v, d_y)	Frequency
(1,2)	1
(1,3)	3
(1,4)	1
(2,2)	1
(2,3)	1
(2,4)	2
(3,3)	2
(3,4)	1

TABLE 9 Vertex and edge partitioning of ribose.

(d_v, d_y)	Frequency
(1,2)	1
(1,3)	3
(2,3)	3
(3,3)	3

TABLE 10 Vertex and edge partitioning of HMP.

(d_v, d_y)	Frequency
(1,2)	3
(1,3)	1
(2,3)	6

$$h(x, y) = \mathbb{M}(\mathcal{CMG}; x, y)$$
$$= (2n+1)xy^2 + (7n+1)xy^3 + 4nx^2y^2 + (14n-1)x^2y^3$$
$$+ 12nx^3y^3,$$

$$\mathcal{D}_x(h(x,y)) = (2n+1)xy^2 + (7n+1)xy^3 + 8nx^2y^2$$
$$+ 2(14n-1)x^2y^3 + 36nx^3y^3, \qquad (22)$$

$$\mathcal{D}_y(h(x,y)) = 2(2n+1)xy^2 + 3(7n+1)xy^3 + 8nx^2y^2$$
$$+ 3(14n-1)x^2y^3 + 36nx^3y^3, \qquad (23)$$

$$\mathcal{D}_x\mathcal{D}_y(h(x,y)) = 2(2n+1)xy^2 + 3(7n+1)xy^3 + 16nx^2y^2$$
$$+ 6(14n-1)x^2y^3 + 108nx^3y^3, \qquad (24)$$

$$\mathcal{S}_x(h(x,y)) = (2n+1)xy^2 + (7n+1)xy^3 + 2nx^2y^2$$
$$+ \frac{1}{2}(14n-1)x^2y^3 + 4nx^3y^3, \qquad (25)$$

$$\mathcal{S}_y\mathcal{S}_x(h(x,y)) = \frac{(2n+1)}{2}xy^2 + \frac{1}{3}(7n+1)xy^3 + 2nx^2y^2$$
$$+ \frac{1}{3}(14n-1)x^2y^3 + 4nx^3y^3, \qquad (26)$$

$$\mathcal{D}_x^\alpha\mathcal{D}_y^\alpha(h(x,y)) = 2^\alpha(2n+1)xy^2 + 3^\alpha(7n+1)xy^3 + 4.2^\alpha.2^\alpha nx^2y^2,$$
$$\qquad (27)$$
$$+ 2^\alpha.3^\alpha(14n-1)x^2y^3 + 12n3^\alpha.3^\alpha x^3y^3, \qquad (28)$$

$$\mathcal{S}_y^\alpha\mathcal{S}_x^\alpha(h(x,y)) = \frac{(2n+1)xy^2}{2^\alpha} + \frac{7n+1}{3^\alpha}xy^3 + \frac{4nx^2y^2}{2^\alpha.2^\alpha}$$
$$+ \frac{14n-1}{2^\alpha.3^\alpha}x^2y^3 + \frac{12nx^3y^3}{3^\alpha.3^\alpha}, \qquad (29)$$

$$\mathcal{S}_y\mathcal{D}_x(h(x,y)) = \frac{(2n+1)xy^2}{2} + \frac{7n+1}{3}xy^3 + 4nx^2y^2$$
$$+ \frac{2}{3}(14n-1)x^2y^3 + 12nx^3y^3, \qquad (30)$$

$$\mathcal{S}_x\mathcal{D}_y(h(x,y)) = 2(2n+1)xy^2 + 3(7n+1)xy^3 + 4nx^2y^2$$
$$+ \frac{3}{2}(14n-1)x^2y^3 + 12nx^3y^3. \qquad (31)$$

TABLE 11 Vertex and edge partitioning of raffinose.

(d_v, d_y)	Frequency
(1,2)	3
(1,3)	8
(2,2)	1
(2,3)	9
(2,4)	3
(3,3)	9
(3,4)	1

From Table 1, we obtain the following equation:

1. $M_1(\Gamma) = \left(\mathcal{D}_x + \mathcal{D}_y\right)\left(\mathbb{M}(\mathcal{CMG}; x, y)\right)|_{x=y=1} = 192n + 1.$

2. $M_2(\Gamma) = \left(\mathcal{D}_x\mathcal{D}_y\right)\left(\mathbb{M}(\mathcal{CMG}; x, y)\right)|_{x=y=1} = 233n - 1.$

3. ${}^mM_2(\Gamma) = \left(\mathcal{S}_x\mathcal{S}_y\right)\left(\mathbb{M}(\mathcal{CMG}; x, y)\right)|_{x=y=1} = 7.99n + 0.663.$

4. $R_\alpha(\Gamma) = \left(\mathcal{D}_x^\alpha\mathcal{D}_y^\alpha\right)\left(\mathbb{M}(\mathcal{CMG}; x, y)\right)|_{x=y=1}$
   $= 2^\alpha(2n+1) + 3^\alpha(7n+1) + 2^{2\alpha+2}n + 2^\alpha3^\alpha(14n-1) + 4.3^{2\alpha+1}n.$

5. $RR_\alpha(\Gamma) = \left(\mathcal{S}_x^\alpha\mathcal{S}_y^\alpha\right)\left(\mathbb{M}(\mathcal{CMG}; x, y)\right)|_{x=y=1}$
   $= \dfrac{1}{2^\alpha}(2n+1) + \dfrac{(7n+1)}{3^\alpha} + \dfrac{n}{2^{2\alpha-2}} + \dfrac{(14n-1)}{2^\alpha3^\alpha} + \dfrac{4n}{3^{2\alpha-1}}.$

6. $SDD(\Gamma) = \left(\mathcal{D}_x\mathcal{S}_y + \mathcal{S}_x\mathcal{D}_y\right)\left(\mathbb{M}(\mathcal{CMG}; x, y)\right)|_{x=y=1} = 90.66n + 3.66.$

Proposition 3.8: *Consider a molecular graph Γ for hydroxypropyl guar and carboxymethyl guar. Then,*

1. $H(\Gamma) = 16.44n + 0.78.$
2. $I(\Gamma) = 45.38n + 0.22.$
3. $AZI(\Gamma) = 320.315n + 3.375.$

Proof: From the edge partitioning of $\mathcal{HPG}$ and $\mathcal{CMG}$ and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equations (Eqs 31–34):

$$h(x, y) = \mathbb{M}(\Gamma; x, y)$$
$$= (2n+1)xy^2 + (7n+1)xy^3 + 4nx^2y^2 + (14n-1)x^2y^3 + 12nx^3y^3,$$

$$I(h(x, y)) = (2n+1)x^3 + (7n+1)x^4 + 4nx^4 + (14n-1)x^5 + 12nx^6, \tag{32}$$

$$S_xI(h(x, y)) = \frac{(2n+1)}{3}x^3 + \frac{(7n+1)}{4}x^4 + nx^4 + \frac{1}{5}(14n-1)x^5 + 2nx^6, \tag{33}$$

$$S_xI\mathcal{D}_x\mathcal{D}_y(h(x, y)) = \frac{2}{3}(2n+1)x^3 + \frac{3(7n+1)}{4}x^4 + 4nx^4 + \frac{6}{5}(14n-1)x^5 + 18nx^6, \tag{34}$$

TABLE 12 Statistical parameters for $H(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 9.133–0.196 $[H(\Gamma)]$	0.222	0.049	0.312	0.597
BP = 506.288–3.227 $[H(\Gamma)]$	0.211	0.045	0.280	0.616
MP = 118.582 + 0.950 $[H(\Gamma)]$	0.276	0.076	0.495	0.508
MW = 243.839 + 0.235 $[H(\Gamma)]$	0.028	0.001	0.005	0.947
WS = 293.061 + 5.979 $[H(\Gamma)]$	0.338	0.114	0.775	0.413
Quadratic regression model				
Density = 0.031 $[H(\Gamma)]^2$-1.944 $[H(\Gamma)]$+19.951	0.394	0.155	0.460	0.656
BP = −1.211 $[H(\Gamma)]^2$ + 65.982 $[H(\Gamma)]$+78.097	0.768	0.590	3.604	0.107
MP = −0.012 $[H(\Gamma)]^2$ + 1.623 $[H(\Gamma)]$+114.412	0.278	0.077	0.209	0.818
MW = −0.885 $[H(\Gamma)]^2$ + 50.800 $[H(\Gamma)]$-69.001	0.988	0.975	99.181	0.0000
WS = 0.660 $[H(\Gamma)]^2$-31.903 $[H(\Gamma)]$+526.307	0.493	0.243	0.803	0.498
Logarithmic regression model				
Density = 18.558–5.507ln $[H(\Gamma)]$	0.333	0.111	0.747	0.421
BP = 441.473 + 10.184ln $[H(\Gamma)]$	0.035	0.001	0.007	0.934
MP = 89.682 + 19.018ln $[H(\Gamma)]$	0.293	0.086	0.563	0.481
MW = 125.979 + 55.510ln $[H(\Gamma)]$	0.352	0.124	0.848	0.393
WS = 234.016 + 62.235ln $[H(\Gamma)]$	0.196	0.037	0.230	0.648

TABLE 13 Statistical parameters for $I(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 15.633–0.514 $[I(\Gamma)]$	0.310	0.096	0.637	0.455
BP = 110.644 + 20.004 $[I(\Gamma)]$	0.691	0.478	5.486	0.058
MP = 108.224 + 1.298 $[I(\Gamma)]$	0.199	0.040	0.248	0.636
MW = −18.121 + 15.020 $[I(\Gamma)]$	0.949	0.901	54.429	0.0000
WS = 549.858–10.212 $[I(\Gamma)]$	0.315	0.099	0.659	0.448
Quadratic regression model				
Density = 0.127 $[I(\Gamma)]^2$-5.501 $[I(\Gamma)]$+55.997	0.347	0.120	0.342	0.726
BP = 1.585 $[I(\Gamma)]^2$-42.153 $[I(\Gamma)]$+613.760	0.700	0.490	2.404	0.186
MP = −2.580 $[I(\Gamma)]^2$ + 102.476 $[I(\Gamma)]$-710.745	0.834	0.696	5.720	0.051
MW = 1.135 $[I(\Gamma)]^2$-29.515 $[I(\Gamma)]$+342.360	0.960	0.922	29.653	0.002
WS = −6.853 $[I(\Gamma)]^2$ + 258.578 $[I(\Gamma)]$-1625.811	0.534	0.285	0.998	0.432
Logarithmic regression model				
Density = 33.404–9.682ln $[I(\Gamma)]$	0.319	0.102	0.679	0.441
BP = −546.406 + 364.277ln $[I(\Gamma)]$	0.688	0.474	5.404	0.059
MP = 48.517 + 29.792ln $[I(\Gamma)]$	0.250	0.063	0.401	0.550
MW = −508.481 + 272.441ln $[I(\Gamma)]$	0.942	0.887	46.901	0.0000
WS = 832.635–166.978ln $[I(\Gamma)]$	0.281	0.079	0.516	0.500

TABLE 14 Statistical parameters for $AZI(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 14.748–0.062 $[AZI(\Gamma)]$	0.355	0.112	0.760	0.417
BP = 143.262 + 2.431 $[AZI(\Gamma)]$	0.752	0.566	7.830	0.031
MP = 128.852 + 0.017 $[AZI(\Gamma)]$	0.024	0.001	0.003	0.956
MW = 15.678 + 1.754 $[AZI(\Gamma)]$	0.993	0.987	443.929	0.0000
WS = 525.992–1.186 $[AZI(\Gamma)]$	0.327	0.107	0.720	0.429
Quadratic regression model				
Density = 0.001 $[AZI(\Gamma)]^2$-0.423 $[AZI(\Gamma)]$+37.145	0.452	0.204	0.642	0.565
BP = 0.015 $[AZI(\Gamma)]^2$-2.284 $[AZI(\Gamma)]$+436.166	0.786	0.618	4.043	0.090
MP = −0.009 $[AZI(\Gamma)]^2$ + 2.815 $[AZI(\Gamma)]$-44.988	0.601	0.361	1.411	0.327
MW = 0.002 $[AZI(\Gamma)]^2$ + 1.081 $[AZI(\Gamma)]$+57.517	0.995	0.990	252.564	0.0000
WS = −0.001 $[AZI(\Gamma)]^2$-0.726 $[AZI(\Gamma)]$+497.430	0.328	0.108	0.301	0.752
Logarithmic regression model				
Density = 56.222–10.460ln $[AZI(\Gamma)]$	0.398	0.159	1.130	0.329
BP = −1074.714 + 323.998ln $[AZI(\Gamma)]$	0.707	0.501	6.012	0.050
MP = 76.730 + 11.456ln $[AZI(\Gamma)]$	0.111	0.012	0.075	0.793
MW = −910.201 + 243.707ln $[AZI(\Gamma)]$	0.973	0.947	107.701	0.0000
WS = 1123.059–158.678ln $[AZI(\Gamma)]$	0.309	0.095	0.633	0.457

TABLE 15 Statistical parameters for $M_1(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 1.375 + 0.002 $[M_1(\Gamma)]$	0.684	0.467	5.261	0.062
BP = 115.600 + 4.200 $[M_1(\Gamma)]$	0.781	0.611	9.413	0.022
MP = 127.371 + 0.045 $[M_1(\Gamma)]$	0.037	0.001	0.008	0.930
MW = 3.754 + 2.934 $[M_1(\Gamma)]$	0.999	0.997	2200.450	0.0000
WS = 522.419–1.844 $[M_1(\Gamma)]$	0.306	0.094	0.619	0.461
Quadratic regression model				
Density = −0.001 $[M_1(\Gamma)]^2$ + 0.0000 $[M_1(\Gamma)]$+1.519	0.706	0.498	2.482	0.178
BP = 0.536 $[M_1(\Gamma)]^2$ + 0.018 $[M_1(\Gamma)]$+262.656	0.789	0.622	4.119	0.088
MP = −0.026 $[M_1(\Gamma)]^2$ + 5.434 $[M_1(\Gamma)]$-88.890	0.705	0.497	2.468	0.180
MW = 0.002 $[M_1(\Gamma)]^2$ + 2.613 $[M_1(\Gamma)]$+16.660	0.999	0.998	1030.398	0.0000
WS = −0.010 $[M_1(\Gamma)]^2$ + 0.252 $[M_1(\Gamma)]$+438.332	0.311	0.097	0.267	0.776
Logarithmic regression model				
Density = 0.729 + 0.193ln $[M_1(\Gamma)]$	0.664	0.441	4.735	0.072
BP = −1125.431 + 369.772ln $[M_1(\Gamma)]$	0.763	0.582	8.360	0.028
MP = 59.381 + 16.694ln $[M_1(\Gamma)]$	0.153	0.023	0.144	0.717
MW = −875.480 + 261.181ln $[M_1(\Gamma)]$	0.986	0.972	204.691	0.0000
WS = 1020.733–151.515ln $[M_1(\Gamma)]$	0.279	0.078	0.505	0.504

$$\mathcal{S}_x^3 \mathcal{Q}_{-2}\mathcal{I}\mathcal{D}_x^3\mathcal{D}_y^3\big(h(x,y)\big) = 8(2n+1)x + \frac{27(7n+1)}{8}x^2 + 32nx^2$$
$$+ 8(14n-1)x^3, \tag{35}$$

$$+\frac{12.27.27}{64}nx^4. \tag{36}$$

From Table 1, we obtain the following equation:

1. $H(\Gamma) = 2(\mathcal{S}_x\mathcal{I})\big(\mathbb{M}(\mathcal{CMG}; x,y)\big)|_{x=1} = 16.44n + 0.78$.
2. $I(\Gamma) = \big(\mathcal{S}_x\mathcal{I}\mathcal{D}_x\mathcal{D}_y\big)\big(\mathbb{M}(\mathcal{CMG}; x,y)\big)|_{x=1} = 45.38n + 0.22$.
3. $AZI(\Gamma) = \big(\mathcal{S}_x^3\mathcal{Q}_{-2}\mathcal{I}\mathcal{D}_x^3\mathcal{D}_y^3\big)\big(\mathbb{M}(\mathcal{CMG}; x,y)\big)|_{x=1} = 320.315n + 3.375$.

3.3 Results for the $\mathcal{CMHPG}$ molecular graph

In the carboxymethyl hydroxypropyl guar molecular graph shown in Figure 6, for the vertices and edges, we obtain the following equation:

$$E_{\{i_0,i_1\}} = \{e = uv \in E(\mathcal{CMHPG}[m,n]): d_u = i_0, d_v = i_1\},$$

such that $|E_{\{1,2\}}| = 3n + 1$, $|E_{\{1,3\}}| = 6n + 1$, $|E_{\{2,2\}}| = 5n$, $|E_{\{2,3\}}| = 15n - 1$, and $|E_{\{3,3\}}| = 12n$.

Theorem 3.10: *Consider a molecular graph Γ for carboxymethyl hydroxypropyl guar. Then,*

$$\mathbb{M}\big(\mathcal{CMHPG}; x,y\big) = (3n+1)xy^2 + (6n+1)xy^3 + 5nx^2y^2$$
$$+ (15n-1)x^2y^3 + 12nx^3y^3.$$

Proof: From the edge partitioning of $\mathcal{CMHPG}$ and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equation:

$$\mathbb{M}\big(\mathcal{CMHPG}; x,y\big) = \sum_{i_0 \le i_1} m_{i_0 j_1}(\Gamma)x^{i_0}y^{i_1}.$$
$$= \sum_{1\le 2} m_{12}(\Gamma)x^1y^2 + \sum_{1\le 3} m_{13}(\Gamma)x^1y^3$$
$$+ \sum_{2\le 2} m_{22}(\Gamma)x^2y^2 + \sum_{2\le 3} m_{22}(\Gamma)x^2y^3$$
$$+ \sum_{3\le 3} m_{33}(\Gamma)x^3y^3.$$
$$= \sum_{uv\in E_{\{1,2\}}} m_{12}(\Gamma)x^1y^2 + \sum_{uv\in E_{\{1,3\}}} m_{13}(\Gamma)x^1y^3 + \sum_{uv\in E_{\{2,2\}}} m_{22}(\Gamma)x^2y^2$$
$$+ \sum_{uv\in E_{\{2,3\}}} m_{23}(\Gamma)x^2y^3 + \sum_{uv\in E_{\{3,3\}}} m_{33}(\Gamma)x^3y^3.$$
$$= |E_{\{1,2\}}|x^1y^2 + |E_{\{1,3\}}|x^1y^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3$$
$$+ |E_{\{3,3\}}|x^3y^3.$$
$$= (3n+1)xy^2 + (6n+1)xy^3 + 5nx^2y^2 + (15n-1)x^2y^3$$
$$+ 12nx^3y^3.$$

Proposition 3.11: *Consider a molecular graph Γ for carboxymethyl hydroxypropyl guar. Then,*

1. $M_1(\Gamma) = 200n + 2$.
2. $M_2(\Gamma) = 242n - 1$.
3. ${}^mM_2(\Gamma) = 8.58n + 0.663$.
4. $R_\alpha(\Gamma) = 2^\alpha(3n+1) + 3^\alpha(6n+1)$

$$+5n.2^{2\alpha} + 2^\alpha 3^\alpha(15n-1) + 12n.3^{2\alpha}.$$

TABLE 16 Statistical parameters for $M_2(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 1.380 + 0.002 $[M_2(\Gamma)]$	0.698	0.487	5.703	0.054
BP = 129.011 + 3.415 $[M_2(\Gamma)]$	0.789	0.622	9.882	0.020
MP = 126.188 + 0.050 $[M_2(\Gamma)]$	0.052	0.003	0.016	0.903
MW = 15.142 + 2.365 $[M_2(\Gamma)]$	0.999	0.999	4276.696	0.0000
WS = 509.284–1.425 $[M_2(\Gamma)]$	0.293	0.086	0.565	0.481
Quadratic regression model				
Density = 0.0000 $[M_2(\Gamma)]^2$ + 0.000 $[M_2(\Gamma)]$+1.473	0.710	0.504	2.538	0.173
BP = 0.008 $[M_2(\Gamma)]^2$ + 1.463 $[M_2(\Gamma)]$+220.317	0.792	0.628	4.220	0.084
MP = −0.018 $[M_2(\Gamma)]^2$ + 4.370 $[M_2(\Gamma)]$-75.841	0.748	0.559	3.169	0.129
MW = 0.001 $[M_2(\Gamma)]^2$ + 2.122 $[M_2(\Gamma)]$+26.541	0.999	0.999	2268.338	0.0000
WS = −0.011 $[M_2(\Gamma)]^2$ + 1.174 $[M_2(\Gamma)]$+387.701	0.307	0.094	0.260	0.781
Logarithmic regression model				
Density = 0.714 + 0.190ln $[M_2(\Gamma)]$	0.690	0.476	5.459	0.058
BP = −1120.210 + 355.799ln $[M_2(\Gamma)]$	0.777	0.604	9.134	0.023
MP = 44.322 + 19.499ln $[M_2(\Gamma)]$	0.189	0.036	0.223	0.654
MW = −849.292 + 246.357ln $[M_2(\Gamma)]$	0.983	0.967	176.423	0.0000
WS = 947.654–129.845ln $[M_2(\Gamma)]$	0.253	0.064	0.410	0.546

5. $RR_\alpha(\Gamma) = \dfrac{1}{2^\alpha}(3n+1) + \dfrac{(6n+1)}{3^\alpha} + \dfrac{5n}{2^{2\alpha}} + \dfrac{(15n-1)}{2^\alpha 3^\alpha} + \dfrac{12n}{3^{2\alpha}}$.

6. $SDD(\Gamma) = 106.03n + 3.66$.

Proof: From the edge partitioning of $\mathcal{CMHPG}$ and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equations (Eqs 35–43):

$$\begin{aligned}\mathcal{J}(x,y) &= \mathbb{M}(\mathcal{CMHPG};x,y)\\ &= (3n+1)xy^2 + (6n+1)xy^3 + 4nx^2y^2 + (15n-1)x^2y^3\\ &\quad + 12nx^3y^3,\end{aligned}$$

$$\begin{aligned}\mathcal{D}_x(\mathcal{J}(x,y)) &= (3n+1)xy^2 + (6n+1)xy^3 + 10nx^2y^2\\ &\quad + 2(15n-1)x^2y^3 + 36nx^3y^3,\end{aligned} \quad (37)$$

$$\begin{aligned}\mathcal{D}_y(\mathcal{J}(x,y)) &= 2(3n+1)xy^2 + 3(6n+1)xy^3 + 10nx^2y^2\\ &\quad + 3(15n-1)x^2y^3 + 36nx^3y^3,\end{aligned} \quad (38)$$

$$\begin{aligned}\mathcal{D}_x\mathcal{D}_y(\mathcal{J}(x,y)) &= 2(3n+1)xy^2 + 3(6n+1)xy^3 + 20nx^2y^2\\ &\quad + 6(15n-1)x^2y^3 + 108nx^3y^3,\end{aligned} \quad (39)$$

$$\begin{aligned}\mathcal{S}_x(\mathcal{J}(x,y)) &= (3n+1)xy^2 + (6n+1)xy^3 + \frac{5}{2}nx^2y^2\\ &\quad + \frac{1}{2}(15n-1)x^2y^3 + 4nx^3y^3,\end{aligned} \quad (40)$$

$$\begin{aligned}\mathcal{S}_y\mathcal{S}_x(\mathcal{J}(x,y)) &= \frac{(3n+1)}{2}xy^2 + \frac{1}{3}(6n+1)xy^3 + \frac{5}{4}nx^2y^2\\ &\quad + \frac{1}{6}(15n-1)x^2y^3 + \frac{4}{3}nx^3y^3,\end{aligned} \quad (41)$$

$$\begin{aligned}\mathcal{D}_x^\alpha\mathcal{D}_y^\alpha(\mathcal{J}(x,y)) &= 2^\alpha(3n+1)xy^2 + 3^\alpha(6n+1)xy^3 + 5.2^\alpha.2^\alpha nx^2y^2\\ &\quad + 2^\alpha.3^\alpha(15n-1)x^2y^3,\end{aligned} \quad (42)$$

$$+12n3^\alpha.3^\alpha x^3y^3, \quad (43)$$

$$\begin{aligned}\mathcal{S}_y^\alpha\mathcal{S}_x^\alpha(\mathcal{J}(x,y)) &= \frac{(3n+1)xy^2}{2^\alpha} + \frac{6n+1}{3^\alpha}xy^3 + \frac{5nx^2y^2}{2^\alpha.2^\alpha}\\ &\quad + \frac{15n-1}{2^\alpha.3^\alpha}x^2y^3 + \frac{12nx^3y^3}{3^\alpha.3^\alpha},\end{aligned} \quad (44)$$

$$\begin{aligned}\mathcal{S}_y\mathcal{D}_x(\mathcal{J}(x,y)) &= \frac{(3n+1)xy^2}{2} + \frac{6n+1}{3}xy^3 + 5nx^2y^2\\ &\quad + \frac{2}{3}(15n-1)x^2y^3 + 12nx^3y^3,\end{aligned} \quad (45)$$

$$\begin{aligned}\mathcal{S}_x\mathcal{D}_y(\mathcal{J}(x,y)) &= 2(3n+1)xy^2 + 3(6n+1)xy^3 + 5nx^2y^2\\ &\quad + \frac{3}{2}(15n-1)x^2y^3 + 12nx^3y^3.\end{aligned} \quad (46)$$

From Table 1, we obtain the following equation:

1. $M_1(\Gamma) = (\mathcal{D}_x + \mathcal{D}_y)(\mathbb{M}(\mathcal{CMHPG};x,y))|_{x=y=1} = 200n + 2$.

2. $M_2(\Gamma) = (\mathcal{D}_x\mathcal{D}_y)(\mathbb{M}(\mathcal{CMHPG};x,y))|_{x=y=1} = 242n - 1$.

3. $^mM_2(\Gamma) = (\mathcal{S}_x\mathcal{S}_y)(\mathbb{M}(\mathcal{CMHPG};x,y))|_{x=y=1} = 8.58n + 0.663$.

4. $R_\alpha(\Gamma) = (\mathcal{D}_x^\alpha\mathcal{D}_y^\alpha)(\mathbb{M}(\mathcal{CMHPG};x,y))|_{x=y=1} = 2^\alpha(3n+1)$

$+3^\alpha(6n+1) + 5n.2^{2\alpha} \qquad + 2^\alpha 3^\alpha(15n-1) + 12n.3^{2\alpha}$.

5. $RR_\alpha(\Gamma) = (\mathcal{S}_x^\alpha\mathcal{S}_y^\alpha)(\mathbb{M}(\mathcal{CMHPG};x,y))|_{x=y=1}$

$= \dfrac{1}{2^\alpha}(3n+1) + \dfrac{(6n+1)}{3^\alpha} + \dfrac{5n}{2^{2\alpha}} + \dfrac{(15n-1)}{2^\alpha 3^\alpha} + \dfrac{12n}{3^{2\alpha}}$.

6. $SDD(\Gamma) = (\mathcal{D}_x\mathcal{S}_y + \mathcal{S}_x\mathcal{D}_y)(\mathbb{M}(\mathcal{CMHPG};x,y))|_{x=y=1}$

$= 106.03n + 3.66$.

TABLE 17 Statistical parameters for $^{m}M_2(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 1.367 + 0.050 $[^{m}M_2(\Gamma)]$	0.665	0.443	4.770	0.072
BP = 90.113 + 98.384 $[^{m}M_2(\Gamma)]$	0.780	0.609	9.335	0.022
MP = 125.904 + 1.375 $[^{m}M_2(\Gamma)]$	0.048	0.02	0.014	0.909
MW = −13.971 + 68.719 $[^{m}M_2(\Gamma)]$	0.997	0.993	905.950	0.0000
WS = 543.926−45.903 $[^{m}M_2(\Gamma)]$	0.325	0.105	0.706	0.433
Quadratic regression model				
Density = 0.013 $[^{m}M_2(\Gamma)]^2$-0.072 $[^{m}M_2(\Gamma)]$+1.593	0.704	0.495	2.451	0.181
BP = −52.840 $[^{m}M_2(\Gamma)]^2$ + 16.606 $[^{m}M_2(\Gamma)]$+369.528	0.798	0.637	4.393	0.079
MP = −14.861 $[^{m}M_2(\Gamma)]^2$ + 136.708 $[^{m}M_2(\Gamma)]$-124.149	0.674	0.454	2.080	0.220
MW = 2.326 $[^{m}M_2(\Gamma)]^2$ + 47.542 $[^{m}M_2(\Gamma)]$+25.157	0.998	0.995	528.816	0.0000
WS = −3.924 $[^{m}M_2(\Gamma)]^2$-10.168 $[^{m}M_2(\Gamma)]$+477.899	0.324	0.107	0.298	0.754
Logarithmic regression model				
Density = 1.313 + 0.199ln $[^{m}M_2(\Gamma)]$	0.640	0.409	4.154	0.088
BP = −17.267 + 391.087ln $[^{m}M_2(\Gamma)]$	0.754	0.569	7.926	0.031
MP = 110.702 + 16.608ln $[^{m}M_2(\Gamma)]$	0.142	0.020	0.124	0.737
MW = −95.851 + 278.575ln $[^{m}M_2(\Gamma)]$	0.983	0.967	177.008	0.0000
WS = 589.578−178.852ln $[^{m}M_2(\Gamma)]$	0.303	0.095	0.627	0.459

Proposition 3.12: *Consider a molecular graph Γ for carboxymethyl hydroxypropyl guar. Then,*

1. $H(\Gamma) = 17.5n + 0.76$
2. $I(\Gamma) = 47.5n + 0.22$
3. $AZI(\Gamma) = 340.95n + 3.4$

Proof: From the edge partitioning of $\mathcal{CMHPG}$ and using the definition $\mathbb{M}$-polynomial of Γ, we obtain the following equations (Eqs 44–47):

$$\mathcal{J}(x, y) = \mathbb{M}(\mathcal{CMPHG}; x, y) = (3n + 1)xy^2 + (6n + 1)xy^3 + 5nx^2y^2$$
$$+ (15n - 1)x^2y^3 + 12nx^3y^3,$$

$$\mathcal{I}(\mathcal{J}(x, y)) = (3n + 1)x^3 + (6n + 1)x^4 + 5nx^4 + (15n - 1)x^5$$
$$+ 12nx^6, \tag{47}$$

$$\mathcal{S}_x\mathcal{I}(\mathcal{J}(x, y)) = \frac{(3n + 1)}{3}x^3 + \frac{(6n + 1)}{4}x^4 + \frac{5}{4}nx^4 + \frac{1}{5}(15n - 1)x^5$$
$$+ 2nx^6, \tag{48}$$

$$\mathcal{S}_x\mathcal{ID}_x\mathcal{D}_y(\mathcal{J}(x, y)) = \frac{2}{3}(3n + 1)x^3 + \frac{3(6n + 1)}{4}x^4 + 5nx^4$$
$$+ \frac{6}{5}(15n - 1)x^5 + 18nx^6, \tag{49}$$

$$\mathcal{S}_x^3\mathcal{Q}_{-2}\mathcal{ID}_x^3\mathcal{D}_y^3(\mathcal{J}(x, y)) = 8(3n + 1)x + \frac{27(6n + 1)}{8}x^2 + 40nx^2$$
$$+ 8(15n - 1)x^3, \tag{50}$$

$$+ \frac{12.27.27}{64}nx^4. \tag{51}$$

From Table 1, we obtain the following equation:

1. $H(\Gamma) = 2(\mathcal{S}_x\mathcal{I})(\mathbb{M}(\mathcal{CMHPG}; x, y))|_{x=1} = 17.5n + 0.76$.
2. $I(\Gamma) = (\mathcal{S}_x\mathcal{ID}_x\mathcal{D}_y)(\mathbb{M}(\mathcal{CMHPG}; x, y))|_{x=1} = 47.5n + 0.22$.
3. $AZI(\Gamma) = (\mathcal{S}_x^3\mathcal{Q}_{-2}\mathcal{ID}_x^3\mathcal{D}_y^3)(\mathbb{M}(\mathcal{CMHPG}; x, y))|_{x=1} = 340.95n + 3.4$.

4 Molecular structures and computations of topological indices for different carbohydrates

Carbohydrates are organic molecules made up of carbon, hydrogen, and oxygen. They come in three main types: monosaccharides, disaccharides, and polysaccharides. These sugars or polymers can be aldehydes or ketones and serve various purposes in various species. Exoskeletons, found on arthropods, are made of chitin, a nitrogen-containing polymer. Guar gum, a non-ionic polysaccharide derived from the cluster bean endosperm, is a new agrochemical. Polysaccharides are polymers formed when several monomer units are linked together through condensation. They are the most common type of biomolecules and are found in various sources, including algal, plant, microbial, and animal sources. The structural parameters of polysaccharides typically define its chemical compositions, molecular weights, molecular

TABLE 18 Statistical parameters for $SDD(\Gamma)$.

Model	r	r^2	F	P
Linear regression model				
Density = 1.361 + 0.005 $[SDD(\Gamma)]$	0.688	0.473	5.388	0.059
BP = 88.568 + 8.898 $[SDD(\Gamma)]$	0.784	0.615	9.587	0.021
MP = 127.401 + 0.088 $[SDD(\Gamma)]$	0.035	0.001	0.007	0.935
MW = −14.123 + 6.193 $[SDD(\Gamma)]$	0.998	0.997	1803.041	0.0000
WS = 530.836–3.824 $[SDD(\Gamma)]$	0.300	0.090	0.596	0.470
Quadratic regression model				
Density = 0.0000 $[SDD(\Gamma)]^2$-0.003 $[SDD(\Gamma)]$+1.521	0.709	0.503	2.529	0.174
BP = 0.077 $[SDD(\Gamma)]^2$ + 0.960 $[SDD(\Gamma)]$+253.757	0.791	0.626	9.194	0.085
MP = −0.115 $[SDD(\Gamma)]^2$ + 11.835 $[SDD(\Gamma)]$-117.049	0.701	0.492	2.420	0.184
MW = 0.005 $[SDD(\Gamma)]^2$ + 5.678 $[SDD(\Gamma)]$-3.409	0.998	0.997	789.458	0.0000
WS = −0.053 $[SDD(\Gamma)]^2$ + 1.594 $[SDD(\Gamma)]$+418.090	0.307	0.094	0.261	0.780
Logarithmic regression model				
Density = 0.798 + 0.209ln $[SDD(\Gamma)]$	0.667	0.445	4.819	0.071
BP = −988.425 + 399.150ln $[SDD(\Gamma)]$	0.765	0.585	8.465	0.027
MP = 69.491 + 16.942ln $[SDD(\Gamma)]$	0.144	0.021	0.128	0.733
MW = −776.633 + 281.361ln $[SDD(\Gamma)]$	0.986	0.973	213.264	0.0000
WS = 951.942–160.064ln $[SDD(\Gamma)]$	0.274	0.075	0.485	0.512

structure, degree of substitution, viscosity, solubility, and particle size, contributing to their structural and chemical properties. These parameters collectively determine the functionality and performance of guar gum in various applications, making it a versatile ingredient in numerous industries. They are highly stable, secure, non-toxic, hydrophilic, and biodegradable as natural biomaterials.

This section examines eight carbohydrate molecules: arabinose, galactose, maltose, sucrose, sorbose, ribose, hydroxymethyl furfural, and raffinose. Their molecular structures are depicted in Figure 7, and their physical and chemical properties are listed in Table 2. Table 3 includes consideration of topological indices through vertex and edge partitioning, as defined in Tables 4–11.

5 Regression models

This section discusses linear, quadratic, and logarithmic regression models. Linear regression predicts the value of one variable based on another, while quadratic models modify variables. Log-regression models linearize variables and test the significance level between topological indices and molecular structures. The mathematical expressions for the linear, quadratic, and logarithmic regression models are as follows:

$$\mathbb{P} = A + B(\mathbb{TI}),$$
$$\mathbb{P} = A + B(\mathbb{TI}) + C(\mathbb{TI})^2,$$
$$\mathbb{P} = A + Bln(\mathbb{TI}).$$

where $\mathbb{P}$ is the property of the molecular structure, A is the constant, B and C are the regression coefficients, and $\mathbb{TI}$ is the topological index. The results of these three regression models for the aforementioned indices are calculated using SPSS statistical software, which are depicted in Tables 12–18.

6 Discussion

A regression model is a statistical technique used to predict the value of a continuous target variable based on input features. Four metrics are crucial in regression analysis: correlation coefficient (r), R-squared (r^2), F-statistic, and p-value. The R-squared value measures how well the independent variables predict the dependent variable, with a higher R-squared indicating a stronger linear relationship. The F-statistic tests the overall significance of the model, with a significant F-statistic indicating a non-zero effect of at least one independent variable on the dependent variable. A small p-value indicates statistical significance, indicating that at least one independent variable has a significant effect on the dependent variable.

This study employs linear, quadratic, and logarithmic regression models to predict five physical and chemical properties of various carbohydrates, considering topological indices as independent and properties as dependent variables. It has been observed that two properties, namely, molecular weight and boiling point, give the best predicted value by each regression model (as the value of R is greater than 0.68 in each case except for linear and logarithmic regressions

of the topological index H). Linear, quadratic, and logarithmic models and their four important metric values are shown in Tables 12–18. The study focuses on the significance of topological descriptors in predicting the molecular structures of gaur gum and its derivatives, which are crucial in predicting the molecular weight of carbohydrates. Quantitative structure–property relationship (QSPR) methodology is a powerful approach used in the field of drug design, material science, environmental chemistry, cheminformatics, and computational chemistry. QSPR methodology focuses on establishing mathematical relationships between the chemical structure of compounds and their properties, allowing for the prediction of properties based on molecular features. One notable difference is that QSPR specifically targets physical and chemical properties of compounds, while QSAR often focuses on biological activities. Additionally, molecular modeling techniques may involve more complex simulations and calculations to predict molecular behavior. Finally, QSPR methodology offers a systematic and quantitative approach to predict physicochemical properties of chemical compounds based on their molecular structure, distinct from other methodologies such as QSAR, MD simulation, DFT, machine learning models, and hybrid QSAR/QSPR models, each with its own advantages and limitations depending on the specific application and research goals.

7 Conclusion

This study focuses on the analysis of the polysaccharide guar gum and its chemical variants, namely, $\mathcal{HPG}$, $\mathcal{CMG}$, and $\mathcal{CMHPG}$. Initially, molecular graphs are used to represent these polysaccharides, and vertex and edge partitions are defined. The closed form of the $\mathbb{M}$-polynomial is then computed for these molecular graphs, using various topological indices such as Zagreb indices, Randić index, inverse Randić index, H index, SDD index, I index, and AZI index. The molecular structures of the four polysaccharides are compared graphically based on these nine degree-based topological indices. It is important to note that polysaccharides are a type of biopolymer and have diverse applications, particularly in food preservation, the pharmaceutical industry, and petroleum extraction. The findings of this research will be valuable for chemists and pharmaceutical researchers in their respective fields of study. The results of this investigation can have various applications in the field of polymer science and material engineering. By analyzing the topological indices of guar gum, researchers can gain insights into its molecular structure, connectivity, and properties. This information can be used to predict and understand the behavior of guar gum in different environments, such as its solubility, viscosity, and interactions with other molecules.

Furthermore, these results can help in the design and optimization of guar gum-based products and formulations. By correlating the topological indices with the performance of guar gum in various applications, researchers can tailor its properties to meet specific requirements in industries such as food, pharmaceuticals, cosmetics, and agriculture. Overall, these results can contribute to a better understanding of its structure–property relationships and facilitate the development of innovative products and technologies in diverse fields.

8 Future work

The authors will investigate the polysaccharide guar gum and its chemical variants with respect to the generalized reverse degree for future work.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material; further inquiries can be directed to the corresponding author.

Author contributions

WK: writing–original draft and writing–review and editing. SY: writing–original draft and writing–review and editing.

Funding

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

References

Ajmal, M., Nazeer, W., Munir, M., Kang, S. M., and Jung, C. Y. (2017). The M-polynomials and topological indices of generalized prism network. *Int. J. Math. analysis* 11 (6), 293–303. doi:10.12988/ijma.2017.7118

Amic, D., Belo, D., Lucic, B., Nikolic, S., and Trinajstic, N. (1998). The vertex-connectivity index revisited. *J. Chem. Inf. Comput. Sci.* 38 (5), 819–822. doi:10.1021/ci980039b

Arockiaraj, M., Greeni, A. B., and Kalaam, A. R. A. (2023b). Comparative analysis of reverse degree and entropy topological indices for drug molecules in blood cancer treatment through QSPR regression models. *Polycycl. Aromat. Compd.*, 1–18. doi:10.1080/10406638.2023.2271648

Arockiaraj, M., Greeni, A. B., and Kalaam, A. R. A. (2023c). Linear versus cubic regression models for analyzing generalized reverse degree based topological indices of certain latest corona treatment drug molecules. *Int. J. Quantum Chem.* 123 (16), e27136. doi:10.1002/qua.27136

Arockiaraj, M., Paul, D., Clement, J., Tigga, S., Jacob, K., and Balasubramanian, K. (2023a). Novel molecular hybrid geometric-harmonic-Zagreb degree based descriptors and their efficacy in QSPR studies of polycyclic aromatic hydrocarbons. *Sar. QSAR Environ. Res.* 34 (7), 569–589. doi:10.1080/1062936x.2023.2239149

Balaban, A. T. (1982). Highly discriminating distance-based topological index. *Chem. Phys. Lett.* 89, 399–404. doi:10.1016/0009-2614(82)80009-2

BeMiller, J. N. (2009). One hundred years of commercial food carbohydrates in the United States. *J. Agric. food Chem.* 57 (18), 8125–8129. doi:10.1021/jf8039236

Bollobs, B., and Erds, P. (1998). Graphs of extremal weights. *Ars Comb.* 50, 225.

Caporossi, G., Gutman, I., Hansen, P., and Pavlovic, L. (2003). Graphs with maximum connectivity index. *Comput. Biol. Chem.* 27 (1), 85–90. doi:10.1016/s0097-8485(02)00016-5

Consonni, V., and Todeschini, R. (2010a). *Molecular descriptors. Recent advances in QSAR studies: methods and applications*, 29–102.

Consonni, V., and Todeschini, R. (2010b). *Molecular descriptors. Recent advances in QSAR studies: methods and applications*. Berlin, Germany: Springer, 29–102.

Das, K. C. (2010). Atom-bond connectivity index of graphs. *Discrete Appl. Math.* 158 (11), 1181–1188. doi:10.1016/j.dam.2010.03.006

Das, K. C., and Gutman, I. (2004). Some properties of the second Zagreb index. *MATCH Commun. Math. Comput. Chem.* 52 (1), 3–1.

Deutsch, E., and Klavar, S. (2014). M-polynomial and degree-based topological indices. Available at: https://arxiv.org/abs/1407.1592.

Estrada, E., Torres, L., Rodriguez, L., and Gutman, I. (1998). An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian J. Chem.* 37A.

Fajtlowicz, S. (1987). On conjectures of Graffiti-II. Congr. *Numer* 60, 187–197.

Favaron, O., Maheo, M., and Sacle, J. F. (1993). Some eigenvalue properties in graphs (conjectures of Graffiti — II). *Discrete Math.* 111 (1-3), 197–220. doi:10.1016/0012-365x(93)90156-n

Furtula, B., Graovac, A., and Vukicevic, D. (2010). Augmented zagreb index. *J. Math. Chem.* 48, 370–380. doi:10.1007/s10910-010-9677-3

Gupta, C. K., Lokesha, V., Shwetha, S. B., and Ranjini, P. S. (2016). On the symmetric division deg index of graph. *Southeast asian Bull. Math.* 40 (1).

Gutman, I., and Das, K. C. (2004). The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem.* 50 (1), 83–92.

Gutman, I., and Furtula, B. (2008). *Recent results in the theory of Randic index*. Kragujevac: Univ. Kragujevac.

Gutman, I., Polansky, O. E., Gutman, I., and Polansky, O. E. (1986). Chemical graphs. *Math. Concepts Org. Chem.*, 19–22. doi:10.1007/978-3-642-70982-1_4

Hovgaard, L., and Brondsted, H. (1996). Current applications of polysaccharides in colon targeting. *Crit. Rev. Ther. drug Carr. Syst.* 13, 185–223. doi:10.1615/critrevtherdrugcarriersyst.v13.i3-4.10

Hu, Y., Li, X., Shi, Y., Xu, T., and Gutman, I. (2005). On molecular graphs with smallest and greatest zeroth-order general Randic index. *MATCH Commun. Math. Comput. Chem.* 54 (2), 425–434.

Kier, L. B., and Hall, L. H. (1976). *Molecular connectivity ill chemistry and drug research*. Amsterdam, Netherlands: Elsevier.

Kier, L. B., and Hall, L. H. (1986). *Molecular connectivity in structure-activity analysis*. Hoboken, New Jersey, United States: Wiley. (No Title).

Li, X., Gutman, I., and Randi, M. (2006). *Mathematical aspects of Randic-type molecular structure descriptors*. Serbia: University of kragujevac, Faculty of Science.

Li, X., and Shi, Y. (2008a). A survey on the Randic index. *MATCH Commun. Math. Comput. Chem.* 59 (1), 127–156.

Li, X., and Shi, Y. (2008b). Some new results on a conjecture about the randic index, mathematical chemistry monographs No. 6. Recent results in the theory of randic index. *Kragujevac*, 57–72.

Milicevic, A., Nikolic, S., and Trinajstic, N. (2004). On reformulated Zagreb indices. *Mol. Divers.* 8, 393–399. doi:10.1023/b:modi.0000047504.14261.2a

Munir, M., Nazeer, W., Rafique, S., and Kang, S. M. (2016a). M-polynomial and related topological indices of nanostar dendrimers. *Symmetry* 8 (9), 97. doi:10.3390/sym8090097

Munir, M., Nazeer, W., Rafique, S., and Kang, S. M. (2016b). M-polynomial and degree-based topological indices of polyhex nanotubes. *Symmetry* 8 (12), 149. doi:10.3390/sym8120149

Munir, M., Nazeer, W., Rafique, S., and Kang, S. M. (2016c). M-polynomial and degree-based topological indices of polyhex nanotubes. *Symmetry* 8 (12), 149. doi:10.3390/sym8120149

Munir, M., Nazeer, W., Shahzadi, Z., and Kang, S. M. (2016d). Some invariants of circulant graphs. *Symmetry* 8 (11), 134. doi:10.3390/sym8110134

Nikolic, S., Kovacevic, G., Milicevic, A., and Trinajstic, N. (2003). The Zagreb indices 30 years after. *Croat. Chem. acta* 76 (2), 113–124.

Prem, D., Singh, S., Gupta, P. P., Singh, J., and Kadyan, S. P. S. (2005). Callus induction and *de novo* regeneration from callus in Guar (Cyamopsis tetragonoloba). *Plant Cell, tissue organ Cult.* 80, 209–214. doi:10.1007/s11240-004-0738-9

Randi, M. (2001). The connectivity index 25 years after. *J. Mol. Graph. Model.* 20 (1), 19–35. doi:10.1016/s1093-3263(01)00098-5

Randi, M. (2008). On history of the Randi index and emerging hostility toward chemical graph theory. *MATCH Commun. Math. Comput. Chem.* 59 (1), 5–124.

Randic, M. (1975). Characterization of molecular branching. *J. Am. Chem. Soc.* 97 (23), 6609–6615. doi:10.1021/ja00856a001

Shanmukha, M. C., Usha, A., Siddiqui, M. K., Fufa, S. A., and Praveen, B. M. (2022). Degree-based molecular descriptors of guar gum and its chemical derivatives. *J. Chem.* 2022, 1–14. doi:10.1155/2022/7371538

Trinajstic, N., Nikolic, S., Milicevic, A., and Gutman, I. (2010). About the zagreb indices. *Kem. u Ind. Cas. Kem. i Kem. Inz. Hrvat.* 59 (12), 577–589.

Vukicevic, D., and Graovac, A. (2004). Valence connectivity versus Randic, Zagreb and modified Zagreb index: a linear algorithm to check discriminative properties of indices in acyclic molecular graphs. *Croat. Chem. acta* 77 (3), 501–508.

Whistler, R. L. (1948). Guar-a new industrial crop. *Chem. Ind.* 62, 60–61.

Whistler, R. L., and Hymowitz, T. (1979). *Guar: agronomy, production, industrial use, and nutrition*. West Lafayette, Indiana, United States: Purdue University Press.

Wiener, H. (1947). Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* 69 (1), 17–20. doi:10.1021/ja01193a005