

Research Article

Degree-Based Topological Indices of Polysaccharides: Amylose and Blue Starch-Iodine Complex

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Starch is a polymer of glucose where alpha-linkages are associated with glucopyranose units. It comprises a mixture of amylose and amylopectin. Furthermore, amylose is a linear chain of hundreds of glucose molecules. Starches are not allowed to be dissolved in water. They can be digested by breaking down alpha bonds (glycosidic bonds). Its cyclic degradation products, called cyclodextrins, are the best role models for amylose. They can be considered simple turns of the amylose propeller that has imploded into a circular path. Both humans and animals have amylases, which allow them to digest starches. The important sources of starch include potatoes, rice, wheat, and maize for human consumption. The production of starches is how plants store glucose. The blue colour of starch produced by an iodine solution or iodine reaction is used for its identification. Polysaccharides with a reduced degree of polymerization, known as dextrans, are produced in the starch's partial acid hydrolysis. Complete hydrolysis leads to glucose. In this article, we compute the topological properties: Zagreb index $M_1(\Gamma)$ and $M_2(\Gamma)$, Randić index $R_\alpha(\Gamma)$ for $\alpha = -(1/2), -1, (1/2), 1$, atom-bond connectivity index $ABC(\Gamma)$, geometric-arithmetic index $GA(\Gamma)$, fourth atom-bond connectivity index $ABC_4(\Gamma)$, fifth geometric-arithmetic index $GA_5(\Gamma)$, and degree-based topological indices of a graph Γ representing polysaccharides, namely, amylose and blue starch-iodine complex. In the end, we compare these indices and depict their graphic behavior.

1. Introduction

Amylose has the most basic structure of all nutritional polysaccharides, composed purely of glucose polymers connected only by $\alpha(1-4)$ bonds. Notice that starch is, in fact, a combination of amylose and amylopectin. Amylose is not allowed to be dissolved in water and is more difficult to digest compared to amylopectin. The complexing of amylopectin with amylose facilitates its water—another view of amylose solubility and digestibility. Amylose plays an important role in the storage of plant energy, and as plants do not require glucose to explode, its dense structure and slow breakdown features are under plant's growth. Another function of polysaccharides within cells refers to structural support. Besides, hemicelluloses are another group of polysaccharides located in plant cell walls.

In 1814, Colin and Claubry discovered the starch-iodine reaction, which is well renowned to any chemist from basic courses in qualitative and quantitative analysis.

The first topological index was derived in 1947 when Wiener worked on the boiling point of paraffin alkanes. It was known as the Wiener number. Later on, it is called a path number. The work [1] described the M-polynomial and degree-based topological indices of graphs. The authors in [2, 3] discussed the symmetric divisor deg index of graphs, first Zagreb after 30 years in changed form and topological indices of molecular structure. The authors in [4] also discussed the π electron energy of hydrocarbons. In recent years, Hasni et al. computed the degree-based topological indices of the line graph of benzene ring embedded in P-type surface in the 2D network [5]. In [6], the authors calculated the index numbers for the edge version of the geometric-

arithmetic index of nanocones. Much research has been done to explain the nature of chromophore absorption at 620 nm that yields starch-iodine complex, the distinctive dark blue colour. Still, there seem to have been many disputes that might be addressed to some extent in recent decades.

Let Γ be connected simple graph with $V(\Gamma)$ a set of vertices and $E(\Gamma)$ a set of edges. Let $u \in V(\Gamma)$ and its degree is represented by \mathfrak{R}_u . The idea of degree-based topological indices began from Wiener index; in 1945, Wiener defined them while studying alkane's boiling point cf. [7]. The first degree-based topological index is Randić index given by Milan Randić in [8] and is described as

$$R_{-(1/2)} = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{R}_u \mathfrak{R}_v}} \quad (1)$$

Generalized Randić index (denoted as $R_\alpha(\Gamma)$) is described as follows:

$$R_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} \left(\mathfrak{R}_u \mathfrak{R}_v \right)^\alpha, \quad \alpha = 1, \frac{1}{2}, -\frac{1}{2}, -1. \quad (2)$$

Inverse generalized Randić index (denoted as $RR_\alpha(\Gamma)$) is described as

$$RR_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\left(\sqrt{\mathfrak{R}_u \mathfrak{R}_v} \right)^\alpha}. \quad (3)$$

In [4, 9, 10], Gutman and Trinajstić introduced and defined the first Zagreb index (denoted as $M_1(\Gamma)$) and second Zagreb index (denoted as $M_2(\Gamma)$) as

$$M_1(\Gamma) = \sum_{uv \in E(\Gamma)} (\mathfrak{R}_u + \mathfrak{R}_v), M_2(\Gamma) = \sum_{uv \in E(\Gamma)} (\mathfrak{R}_u \mathfrak{R}_v). \quad (4)$$

In [11], Estrada introduced and studied about the atom-bond connectivity index (denoted as $ABC(\Gamma)$). It is defined as follows:

$$ABC(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{\mathfrak{R}_u + \mathfrak{R}_v - 2}{\mathfrak{R}_u \mathfrak{R}_v}}. \quad (5)$$

Geometric-arithmetic index (denoted as $GA(\Gamma)$) was given by Vukičević cf. [12] and is defined as follows:

$$GA(\Gamma) = \sum_{uv \in E(\Gamma)} 2 \frac{\sqrt{\mathfrak{R}_u \mathfrak{R}_v}}{\mathfrak{R}_u + \mathfrak{R}_v}. \quad (6)$$

The fourth version of the ABC index (denoted as $ABC_4(\Gamma)$) was introduced by Ghorbani in [13] and is defined as

$$ABC_4(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}, \quad (7)$$

where $S_u = \sum_{v=N_\Gamma(u)} \mathfrak{R}_v$ and $N_\Gamma(u) = \{v \in V(\Gamma) | uv \in E(\Gamma)\}$.

The fifth version of the GA index (denoted as $GA_5(\Gamma)$) was given by Graovac cf. [14] and is defined as

$$GA_5(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \quad (8)$$

2. Result for Amylose

Starch is a polymer of glucose whose glucopyranose alpha bonds bind cells. It is a mixture of amylose and amylopectin. Amylose is a linear chain of hundreds of glucose molecules. Starches cannot be dissolved in water. They can be digested by breaking the alpha bonds (glycosidic bonds). Amylose is a polysaccharide composed of α -D-glucose units, linked by $\alpha(1-4)$ glycosidic bonds. It is one of the two starch components that make up about 20 to 30 percent. Due to its tight spiral structure, amylose seems to be more resilient to digestion than other starch molecules and is, thus, a significant form of resistant starch [15] (see Figure 1 for a molecular structure of amylose and Figure 2 for its unit graph and the graph model corresponding to amylose for $n=4$, where n is the number of units). In amylose, there are three types of vertices having degrees 1, 2, and 3. For $n \geq 2$, amylose has four types of edge partitions as

$$\begin{aligned} E_{1,2}(\Gamma) &= \{ \mathfrak{R}_u = 1, \mathfrak{R}_v = 2 \text{ and } u, v \in V(\Gamma) \}, \\ E_{1,3}(\Gamma) &= \{ \mathfrak{R}_u = 1, \mathfrak{R}_v = 3 \text{ and } u, v \in V(\Gamma) \}, \\ E_{2,3}(\Gamma) &= \{ \mathfrak{R}_u = 2, \mathfrak{R}_v = 3 \text{ and } u, v \in V(\Gamma) \}, \\ E_{3,3}(\Gamma) &= \{ \mathfrak{R}_u = 3, \mathfrak{R}_v = 3 \text{ and } u, v \in V(\Gamma) \}. \end{aligned} \quad (9)$$

Theorem 1. For all $n \geq 2$, let Γ be the graph of amylose, then we have the following:

$$\begin{aligned} R_1(\Gamma) &= 74n - 6, \\ R_{(1/2)}(\Gamma) &= 29.1258n - 1.4349, \\ R_{-(1/2)}(\Gamma) &= 5.2363n + 0.3382, \\ R_{-1}(\Gamma) &= 2.4444n + 0.3334. \end{aligned} \quad (10)$$

Proof. The general Randić connectivity index $R_\alpha(\Gamma)$ for $\alpha = 1$ is

$$R_1(\Gamma) = \sum_{uv \in E(\Gamma)} \mathfrak{R}_u \mathfrak{R}_v. \quad (11)$$

From Table 1 and equation (2), we get

$$\begin{aligned} R_1(\Gamma) &= n(1 \times 2) + (2n + 2)(1 \times 3) + (5n - 2)(2 \times 3) \\ &\quad + 4n(3 \times 3) = 74n - 6. \end{aligned} \quad (12)$$

Now, for $\alpha = (1/2)$, the general Randić connectivity index $R_\alpha(\Gamma)$ is

$$R_{(1/2)}(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\mathfrak{R}_u \mathfrak{R}_v}. \quad (13)$$

Again, from Table 1 and equation (2), we have

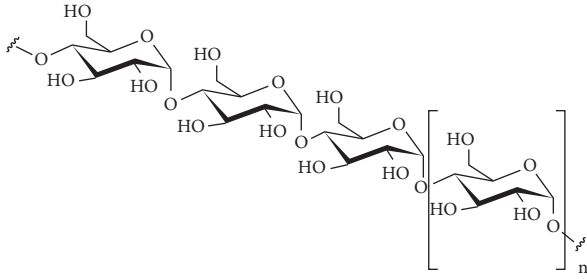


FIGURE 1: Molecular structure of amylose.

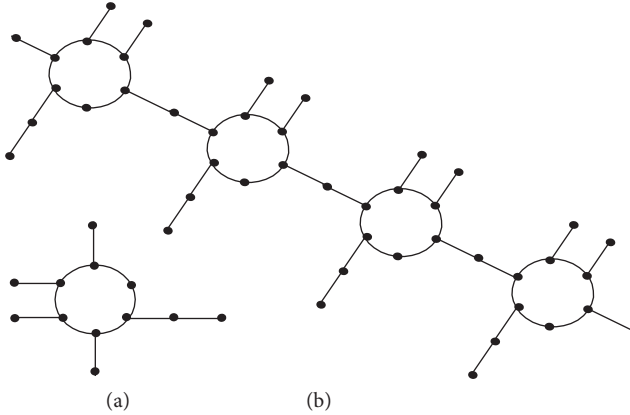
FIGURE 2: (a) Graph of amylose for $n = 1$ and (b) graph of amylose for $n = 4$.

TABLE 1: Edge partition of edges based on the degree of vertices.

Types of edges	$E_{\{1,2\}}$	$E_{\{1,3\}}$	$E_{\{2,3\}}$	$E_{\{3,3\}}$
Edges	(1, 2)	(1, 3)	(2, 3)	(3, 3)
Frequency	n	$2n + 2$	$5n - 2$	$4n$

$$R_{(1/2)}(\Gamma) = n\sqrt{(1 \times 2)} + (2n + 2)\sqrt{(1 \times 3)} + (5n - 2)\sqrt{(2 \times 3)} + 4n\sqrt{(3 \times 3)} \quad (14)$$

$$= 29.1258n - 1.4349.$$

If $\alpha = -(1/2)$, then

$$R_{-(1/2)}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{R}_u \mathfrak{R}_v}} \quad (15)$$

From Table 1 and equation (2), it follows that

$$R_{-(1/2)}(\Gamma) = \frac{n}{\sqrt{(1 \times 2)}} + \frac{(2n + 2)}{\sqrt{(1 \times 3)}} + \frac{(5n - 2)}{\sqrt{(2 \times 3)}} + \frac{4n}{\sqrt{(3 \times 3)}} \quad (16)$$

$$= 5.2363n + 0.3382.$$

Now, for $\alpha = -1$, we have

$$R_{-1}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\mathfrak{R}_u \mathfrak{R}_v} \quad (17)$$

From Table 1 and equation (2), we get

$$R_{-1}(\Gamma) = \frac{n}{(1 \times 2)} + \frac{(2n + 2)}{(1 \times 3)} + \frac{(5n - 2)}{(2 \times 3)} + \frac{4n}{(3 \times 3)} \quad (18)$$

$$= 2.4444n + 0.3334. \quad \square$$

Theorem 2. For all $n \geq 2$, let Γ be the graph of amylose, then, we have the following:

$$M_1(\Gamma) = 60n - 2,$$

$$M_2(\Gamma) = 74n - 6,$$

$$ABC(\Gamma) = 8.5423n + 0.2188,$$

$$GA(\Gamma) = 11.5738n - 0.2276. \quad (19)$$

Proof. By using Table 1 and equation (4), we get

$$M_1(\Gamma) = \sum_{uv \in E(\Gamma)} (\mathfrak{R}_u + \mathfrak{R}_v)$$

$$= n(1 + 2) + (2n + 2)(1 + 3) + (5n - 2)(2 + 3) + 4n(3 + 3)$$

$$= 60n - 2,$$

$$M_2(\Gamma) = \sum_{uv \in E(\Gamma)} \mathfrak{R}_u \mathfrak{R}_v$$

$$= n(1 \times 2) + (2n + 2)(1 \times 3) + (5n - 2)(2 \times 3) + 4n(3 \times 3)$$

$$= 74n - 6.$$

$$M_2(\Gamma) = \sum_{uv \in E(\Gamma)} \widetilde{\mathfrak{R}_u} \widetilde{\mathfrak{R}_v}$$

$$= n(1 \times 2) + (2n + 2)(1 \times 3) + (5n - 2)(2 \times 3) + 4n(3 \times 3)$$

$$= 74n - 6. \quad (20)$$

By using Table 1 and equation (5), we get

$$ABC(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{\mathfrak{R}_u + \mathfrak{R}_v - 2}{\mathfrak{R}_u \mathfrak{R}_v}}$$

$$= n\sqrt{\frac{1 + 2 - 2}{1 \times 2}} + (2n + 2)\sqrt{\frac{1 + 3 - 2}{1 \times 3}} \quad (21)$$

$$+ (5n - 2)\sqrt{\frac{2 + 3 - 2}{2 \times 3}} + 4n\sqrt{\frac{3 + 3 - 2}{3 \times 3}}$$

$$= 8.5423n + 0.2188.$$

By using Table 1 and equation (6), we get

$$\begin{aligned}
 GA(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\mathfrak{R}_u \mathfrak{R}_v}}{\mathfrak{R}_u + \mathfrak{R}_v} \\
 &= 2 \left(n \frac{\sqrt{1 \times 2}}{(1+2)} + (2n+2) \frac{\sqrt{1 \times 3}}{(1+3)} \right. \\
 &\quad \left. + (5n-2) \frac{\sqrt{2 \times 3}}{(2+3)} + 4n \frac{\sqrt{3 \times 3}}{(3+3)} \right) \\
 &= 11.5738n - 0.2276.
 \end{aligned} \tag{22}$$

In Table 2, we give the edge partition centered on degree sum of end vertices for each edge. \square

Theorem 3. For all $n \geq 2$, let Γ be the graph of amylose, then we have

$$\begin{aligned}
 ABC_4(\Gamma) &= 6.4972n + 0.2874, \\
 GA_5(\Gamma) &= 11.7142n - 0.123.
 \end{aligned} \tag{23}$$

Proof. By using Table 2 and equation (7), we get

$$\begin{aligned}
 ABC_4(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\
 &= n \sqrt{\frac{2+4-2}{2 \times 4}} + \sqrt{\frac{3+6-2}{3 \times 6}} + (2n+1) \sqrt{\frac{3+7-2}{3 \times 7}} + n \sqrt{\frac{4+7-2}{4 \times 7}} + \sqrt{\frac{6+6-2}{6 \times 6}} \\
 &\quad + (3n-1) \sqrt{\frac{6+7-2}{6 \times 7}} + (n-1) \sqrt{\frac{6+8-2}{6 \times 8}} + (2n+1) \sqrt{\frac{7+7-2}{7 \times 7}} + (2n-2) \sqrt{\frac{7+8-2}{7 \times 8}} \\
 &= 6.4972n + 0.2874.
 \end{aligned} \tag{24}$$

By using Table 2 and equation (8), we get

$$\begin{aligned}
 GA_5(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \\
 &= 2 \left(n \frac{\sqrt{2 \times 4}}{(2+4)} + \frac{\sqrt{3 \times 6}}{(3+6)} + (2n+1) \frac{\sqrt{3 \times 7}}{(3+7)} + n \frac{\sqrt{4 \times 7}}{(4+7)} + \frac{\sqrt{6 \times 6}}{(6+6)} + (3n-1) \frac{\sqrt{6 \times 7}}{(6+7)} \right. \\
 &\quad \left. + (n-1) \frac{\sqrt{6 \times 8}}{(6+8)} + (2n+1) \frac{\sqrt{7 \times 7}}{(7+7)} + (2n-2) \frac{\sqrt{7 \times 8}}{(7+8)} \right) \\
 &= 11.7142n - 0.123.
 \end{aligned} \tag{25}$$

\square

3. Numerical and Graphical Representation

The numeric representation of the results calculated above is illustrated in Tables 3 and 4, while the graphic representation is devoted to Figures 3 and 4.

4. Results for Blue Starch-Iodine Complex

The main structure of amylose are cyclic degradants known as cyclodextrins. They are obtained enzymatically and may be considered as single turns of the helix of amylose imploding into a circular path. In all of these complexes, cyclodextrin molecules are positioned in

front to form dimers and they are piled together to generate large cylinders that resemble the amylose helix in its global structure. The most interesting one is (trimesic acid H_2O)₁₀HI₅ with linear polyiodide chain. This structural model was accepted, but, unfortunately, cannot shed light on the actual configuration of the polyiodide chain (see Figure 5 for the molecular structure of blue starch-iodine and Figure 6 for its unit graph and the graph model corresponding to blue starch-iodine for $n=6$, where n is the number of units). In starch-iodine, there are three types of vertices having degrees 1, 2, and 3. For $n \geq 3$, blue starch-iodine complex has five types of edge partitions as

TABLE 2: Edge partition based on the degree sum of end vertices of each edge.

Types of edges	$E_{\{2,4\}}$	$E_{\{3,6\}}$	$E_{\{3,7\}}$	$E_{\{4,7\}}$	$E_{\{6,6\}}$	$E_{\{6,7\}}$	$E_{\{6,8\}}$	$E_{\{7,7\}}$	$E_{\{7,8\}}$
Number of edges	(2, 4)	(3, 6)	(3, 7)	(4, 7)	(6, 6)	(6, 7)	(6, 8)	(7, 7)	(7, 8)
Frequency	n	1	$2n + 1$	n	1	$3n - 1$	$n - 1$	$2n + 1$	$2n - 2$

TABLE 3: Numerical comparison of $M_1(\Gamma)$, $M_2(\Gamma)$, $ABC(\Gamma)$, $GA(\Gamma)$, $R_1(\Gamma)$, $R_{-1}(\Gamma)$, $R_{(1/2)}(\Gamma)$, and $R_{-(1/2)}(\Gamma)$.

n	$M_1(\Gamma)$	$M_2(\Gamma)$	$ABC(\Gamma)$	$GA(\Gamma)$	$R_1(\Gamma)$	$R_{-1}(\Gamma)$	$R_{(1/2)}(\Gamma)$	$R_{-(1/2)}(\Gamma)$
1	58	68	8.7611	11.3462	68	2.7778	27.6909	5.5746
2	118	142	17.3034	22.92	142	5.2222	56.8166	10.8109
3	178	216	25.8457	34.4938	216	7.6667	85.9424	16.0474
4	238	290	34.388	46.0676	290	10.1111	115.0682	21.2837
5	298	364	42.9303	57.6414	364	12.5556	144.1939	26.5201
6	358	438	51.4726	69.2152	438	15	173.3197	31.7565
7	418	512	60.0149	80.789	512	17.4444	202.4455	36.9929
8	478	586	68.5572	92.3628	586	19.8889	231.5712	42.2293
9	538	660	77.0995	103.9366	660	22.3333	260.6969	47.4656
10	598	734	85.6418	115.5104	734	24.7778	289.8228	52.7020

TABLE 4: Numerical comparison of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$.

n	1	2	3	4	5	6	7	8	9	10
$ABC_4(\Gamma)$	6.785	13.282	19.779	26.276	32.773	39.271	45.768	52.265	58.762	65.259
$GA_5(\Gamma)$	11.591	23.305	35.019	46.734	58.448	70.162	81.876	93.5906	105.305	117.019

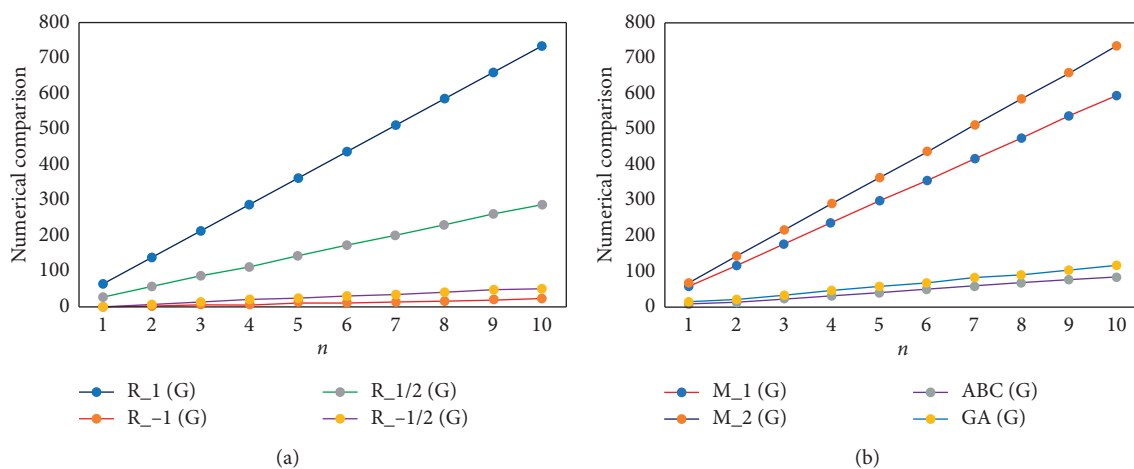
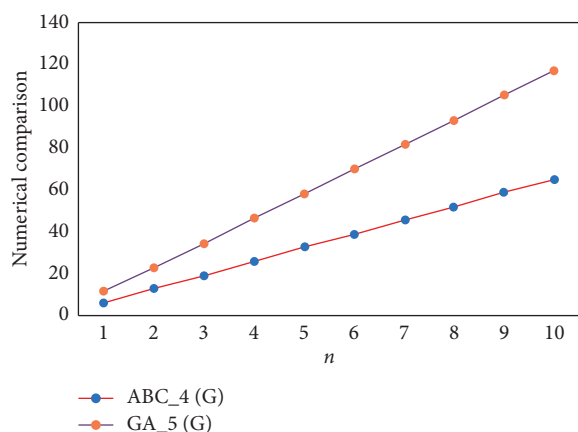
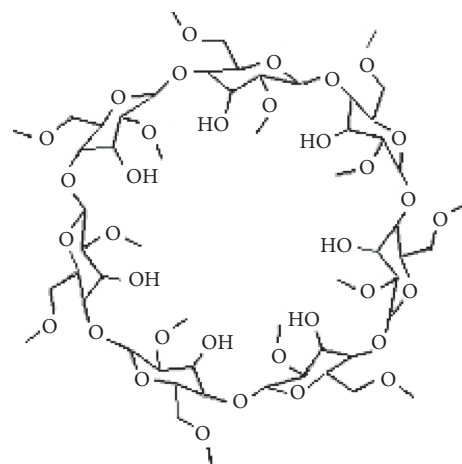
FIGURE 3: (a) Comparison of R_α for $\alpha = 1, -1, (1/2), -(1/2)$ and (b) comparison of $M_1(\Gamma)$, $M_2(\Gamma)$, $ABC(\Gamma)$, and $GA(\Gamma)$ FIGURE 4: Comparison of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$ 

FIGURE 5: Molecular structure of blue starch-iodine.

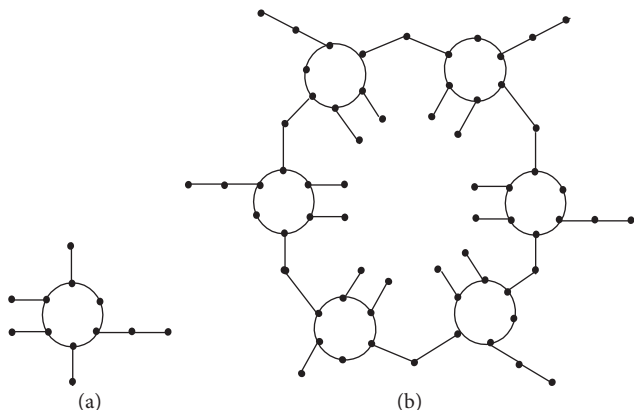


FIGURE 6: (a) Graph of blue starch-iodine for $n = 1$ and (b) graph of blue starch-iodine for $n = 6$.

$$\begin{aligned}
 E_{1,2}(\Gamma) &= \{\widetilde{\mathfrak{R}}_u = 1, \widetilde{\mathfrak{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}, \\
 E_{1,3}(\Gamma) &= \{\widetilde{\mathfrak{R}}_u = 1, \widetilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}, \\
 E_{2,2}(\Gamma) &= \{\widetilde{\mathfrak{R}}_u = 2, \widetilde{\mathfrak{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}, \\
 E_{2,3}(\Gamma) &= \{\widetilde{\mathfrak{R}}_u = 2, \widetilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}, \\
 E_{3,3}(\Gamma) &= \{\widetilde{\mathfrak{R}}_u = 3, \widetilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}.
 \end{aligned} \quad (26)$$

Theorem 4. For all $n \geq 3$, let Γ be the graph of blue starch-iodine complex, we have the following $R_\alpha(\Gamma)$, $\alpha \in R$:

$$\begin{aligned}
 R_1(\Gamma) &= 39n^2 - n + 12, \\
 R_{(1/2)}(\Gamma) &= 16.429n^2 - 1.0354 + 2.8695, \\
 R_{-(1/2)}(\Gamma) &= 3.0272n^2 + .5585n - 0.6764, \\
 R_{-1}(\Gamma) &= 0.75n^2 + 0.6944n - 0.6667.
 \end{aligned} \quad (27)$$

Proof. For $\alpha = 1$, the general Randić connectivity index is

$$R_1(\Gamma) = \sum_{uv \in E(\Gamma)} \widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v. \quad (28)$$

From Table 5 (for edge partition) and equation (2), we get

$$\begin{aligned}
 R_1(\Gamma) &= 2n(1 \times 2) + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] (1 \times 3) \\
 &\quad + n(2 \times 2) + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] (2 \times 3) + 4n(3 \times 3) \\
 &= 39n^2 - n + 12.
 \end{aligned} \quad (29)$$

Now, for $\alpha = (1/2)$, we have

$$R_{(1/2)}(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}. \quad (30)$$

By using Table 5 and equation (2), after simplification, we have

$$\begin{aligned}
 R_{(1/2)}(\Gamma) &= 2n\sqrt{(1 \times 2)} + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] \sqrt{(1 \times 3)} \\
 &\quad + n\sqrt{(2 \times 2)} + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] \sqrt{(2 \times 3)} \\
 &\quad + 4n\sqrt{(3 \times 3)} \\
 &= 16.429n^2 - 1.0354 + 2.8695.
 \end{aligned} \quad (31)$$

For $\alpha = -(1/2)$, we have

$$R_{-(1/2)}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}} \quad (32)$$

From Table 5 and equation (2), it follows that

$$\begin{aligned}
 R_{-(1/2)}(\Gamma) &= \frac{2n}{\sqrt{(1 \times 2)}} + \frac{\left[\sum_{i=1}^{n-1} (n+2) - 2 \right]}{\sqrt{(1 \times 3)}} \\
 &\quad + \frac{n}{\sqrt{(2 \times 2)}} + \frac{\left[\sum_{i=1}^{n-1} (6n-2) + 2 \right]}{\sqrt{(2 \times 3)}} + \frac{4n}{\sqrt{(3 \times 3)}} \\
 &= 3.0272n^2 + .5585n - 0.6764.
 \end{aligned} \quad (33)$$

For $\alpha = -1$, we have

$$R_{-1}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}. \quad (34)$$

Again by using Table 5 and equation (2), we get

$$\begin{aligned}
 R_{-1}(\Gamma) &= \frac{2n}{(1 \times 2)} + \frac{\left[\sum_{i=1}^{n-1} (n+2) - 2 \right]}{(1 \times 3)} + \frac{n}{(2 \times 2)} \\
 &\quad + \frac{\left[\sum_{i=1}^{n-1} (6n-2) + 2 \right]}{(2 \times 3)} + \frac{4n}{(3 \times 3)} \\
 &= 0.75n^2 + 0.6944n - 0.6667.
 \end{aligned} \quad (35)$$

□

Theorem 5. For all $n \geq 3$, let Γ be the graph of blue starch-iodine complex, then we have the following:

$$\begin{aligned}
 M_1(\Gamma) &= 34n^2 - 2n + 4, \\
 M_2(\Gamma) &= 39n^2 - n + 12, \\
 ABC(\Gamma) &= 5.0591n^2 - 0.0523n - 0.4376, \\
 GA(\Gamma) &= 6.7448n^2 - 3.0868n + 0.4552.
 \end{aligned} \quad (36)$$

Proof. By using Table 5 and equation (4), we get

TABLE 5: Edge partition based on the degree of vertices.

Types of edges	$E_{\{1,2\}}$	$E_{\{1,3\}}$	$E_{\{2,2\}}$	$E_{\{2,3\}}$	$E_{\{3,3\}}$
Number of edges	(1, 2)	(1, 3)	(2, 2)	(2, 3)	(3, 3)
Frequency	$2n$	$\sum_{i=1}^{n-1} (n+2) - 2$	n	$\sum_{i=1}^{n-1} (6n-2) + 2$	$4n$

$$\begin{aligned}
M_1(\Gamma) &= \sum_{uv \in E(\Gamma)} (\overline{\mathfrak{R}}_u + \overline{\mathfrak{R}}_v) \\
&= 2n(1+2) + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] (1+3) + n(2+2) \\
&\quad + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] (2+3) + 4n(3+3) \\
&= 34n^2 - 2n + 4, \\
M_2(\Gamma) &= \sum_{uv \in E(\Gamma)} \overline{\mathfrak{R}}_u \overline{\mathfrak{R}}_v \\
&= 2n(1 \times 2) + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] (1 \times 3) + n(2 \times 2) \\
&\quad + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] (2 \times 3) + 4n(3 \times 3) \\
&= 39n^2 - n + 12.
\end{aligned} \tag{37}$$

TABLE 6: Edge partition based on the degree sum of end vertices of each edge.

Types of edges	No. of edges	Frequency
$E_{\{2,3\}}$	(2, 3)	n
$E_{\{2,4\}}$	(2, 4)	n
$E_{\{3,5\}}$	(3, 5)	n
$E_{\{3,6\}}$	(3, 6)	$\sum_{i=1}^{n-1} (1) - 1$
$E_{\{3,7\}}$	(3, 7)	$\sum_{i=1}^{n-1} (n) - 1$
$E_{\{4,8\}}$	(4, 8)	n
$E_{\{5,7\}}$	(5, 7)	n
$E_{\{6,6\}}$	(6, 6)	$\sum_{i=1}^{n-1} (1) - 1$
$E_{\{6,7\}}$	(6, 7)	$\sum_{i=1}^{n-1} (3n-2) + 2$
$E_{\{6,8\}}$	(6, 8)	n
$E_{\{7,7\}}$	(7, 7)	$\sum_{i=1}^{n-1} (2) - 2$
$E_{\{7,8\}}$	(7, 8)	$\sum_{i=1}^{n-1} (4n-3) + 3$

By using Table 5 and equation (5), we get

$$\begin{aligned}
ABC(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{\overline{\mathfrak{R}}_u + \overline{\mathfrak{R}}_v - 2}{\overline{\mathfrak{R}}_u \overline{\mathfrak{R}}_v}} \\
&= 2n \sqrt{\frac{1+2-2}{1 \times 2}} + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] \sqrt{\frac{1+3-2}{1 \times 3}} + n \sqrt{\frac{2+2-2}{2 \times 2}} + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] \sqrt{\frac{2+3-2}{2 \times 3}} \\
&\quad + 4n \sqrt{\frac{3+3-2}{3 \times 3}} \\
&= 5.0591n^2 - 0.0523n - 0.4376.
\end{aligned} \tag{38}$$

By using Table 5 and equation (6), we get

$$\begin{aligned}
GA(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\overline{\mathfrak{R}}_u \overline{\mathfrak{R}}_v}}{(\overline{\mathfrak{R}}_u + \overline{\mathfrak{R}}_v)} \\
&= 2 \left(2n \frac{\sqrt{1 \times 2}}{(1+2)} + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] \frac{\sqrt{1 \times 3}}{(1+3)} + n \frac{\sqrt{2 \times 2}}{(2+2)} + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] \frac{\sqrt{2 \times 3}}{(2+3)} + 4n \frac{\sqrt{3 \times 3}}{(3+3)} \right) \\
&= 6.7448n^2 - 3.0868n + 0.4552.
\end{aligned} \tag{39}$$

□

TABLE 7: Numerical comparison of $M_1(\Gamma)$, $M_2(\Gamma)$, $ABC(\Gamma)$, $GA(\Gamma)$, $R_1(\Gamma)$, $R_{-1}(\Gamma)$, $R_{(1/2)}(\Gamma)$, and $R_{-(1/2)}(\Gamma)$.

n	$M_1(\Gamma)$	$M_2(\Gamma)$	$ABC(\Gamma)$	$GA(\Gamma)$	$R_1(\Gamma)$	$R_{-1}(\Gamma)$	$R_{(1/2)}(\Gamma)$	$R_{-(1/2)}(\Gamma)$
1	36	50	4.5692	4.1132	50	1.361	18.2633	2.9093
2	136	166	19.6942	21.2608	166	6.0553	66.5148	12.5488
3	304	360	44.9374	51.898	360	13.4162	147.6243	28.2419
4	540	632	80.2988	96.0248	632	23.4437	261.5918	49.9887
5	844	982	125.7784	153.6412	982	36.1378	408.4173	77.7891
6	1216	1410	181.3762	224.7472	1410	51.4985	588.1007	111.6433
7	1656	1916	247.0922	309.3428	1916	69.5258	800.6421	151.5512
8	2164	2500	322.9264	407.428	2500	90.2197	1046.0415	197.5126
9	2740	3162	408.8788	519.0028	3162	113.5802	1324.2989	249.5278
10	3384	3902	504.9494	644.0672	3902	139.6073	1635.4143	307.5967

TABLE 8: Numerical comparison of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$.

n	1	2	3	4	5	6	7	8	9	10
$ABC_4(\Gamma)$	3.35	14.82	34.45	62.24	98.19	142.30	194.57	255	323.59	400.34
$GA_5(\Gamma)$	5.94	26.49	62.86	115.02	182.97	266.72	366.27	481.62	612.76	759.70

Theorem 6. For all $n \geq 3$, let Γ be the graph of blue starch-iodine complex, we have

$$\begin{aligned} ABC_4(\Gamma) &= 4.0798n^2 - 0.7682n + 0.04, \\ GA_5(\Gamma) &= 7.8987n^2 - 3.1339n + 1.1727. \end{aligned} \quad (40)$$

Proof. By using Table 6 and equation (7), we get

$$\begin{aligned} ABC_4(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\ &= n\sqrt{\frac{2+3-2}{2 \times 3}} + n\sqrt{\frac{2+4-2}{2 \times 4}} + n\sqrt{\frac{3+5-2}{3 \times 5}} + (n-2)\sqrt{\frac{3+6-2}{3 \times 6}} + (n^2 - n - 1)\sqrt{\frac{3+7-2}{3 \times 7}} \\ &\quad + n\sqrt{\frac{4+8-2}{4 \times 8}} + n\sqrt{\frac{5+7-2}{5 \times 7}} + (n-2)\sqrt{\frac{6+6-2}{6 \times 6}} + (3n^2 - 5n + 4)\sqrt{\frac{6+7-2}{6 \times 7}} \\ &\quad + n\sqrt{\frac{6+8-2}{6 \times 8}} + (2n-4)\sqrt{\frac{7+7-2}{7 \times 7}} + (4n^2 - 7n + 6)\sqrt{\frac{7+8-2}{7 \times 8}} \\ &= 4.0798n^2 - 0.7682n + 0.04. \end{aligned} \quad (41)$$

By using Table 6 and equation (8), we get

$$\begin{aligned} GA_5(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)} \\ &= 2\left(n \frac{\sqrt{2 \times 3}}{(2+3)} + n \frac{\sqrt{2 \times 4}}{(2+4)} + n \frac{\sqrt{3 \times 5}}{(3+5)} + (n-2) \frac{\sqrt{3 \times 6}}{(3+6)} + (n^2 - n - 1) \frac{\sqrt{3 \times 7}}{(3+7)} + n \frac{\sqrt{4 \times 8}}{(4+8)} + n \frac{\sqrt{5 \times 7}}{(5+7)}\right) \\ &\quad + (n-2) \frac{\sqrt{6 \times 6}}{(6+6)} + (3n^2 - 5n + 4) \frac{\sqrt{6 \times 7}}{(6+7)} + n \frac{\sqrt{6 \times 8}}{(6+8)} + (2n-4) \frac{\sqrt{7 \times 7}}{(7+7)} + (4n^2 - 7n + 6) \frac{\sqrt{7 \times 8}}{(7+8)} \\ &= 7.8987n^2 - 3.1339n + 1.1727. \end{aligned} \quad (42)$$

□

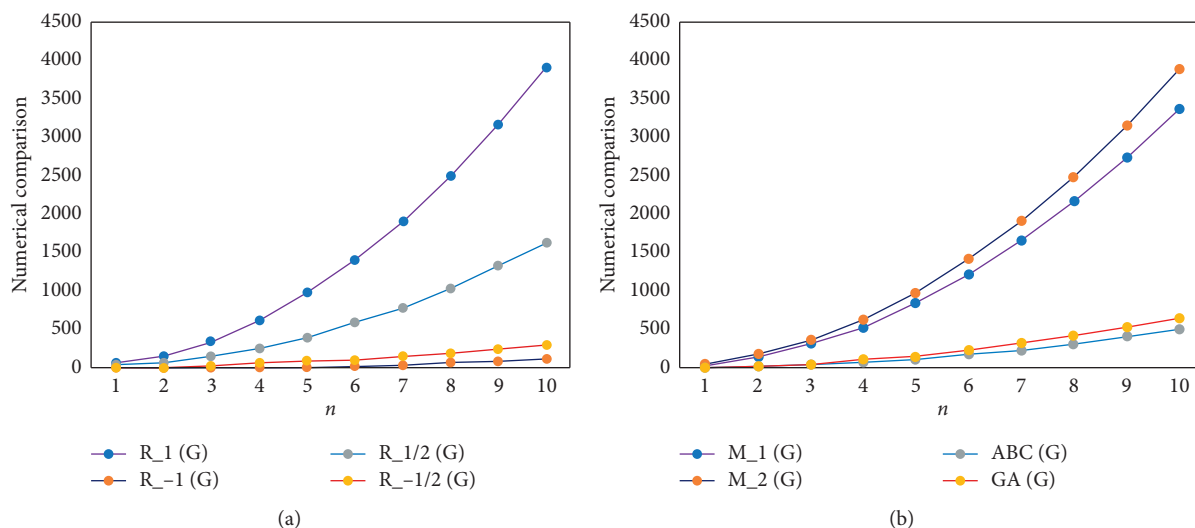


FIGURE 7: (a) Comparison of $R_\alpha(\Gamma)$ for 1, -1, (1/2), -(1/2) and (b) comparison of $M_1(\Gamma)$, $M_2(\Gamma)$, $ABC(\Gamma)$, and $GA(\Gamma)$.

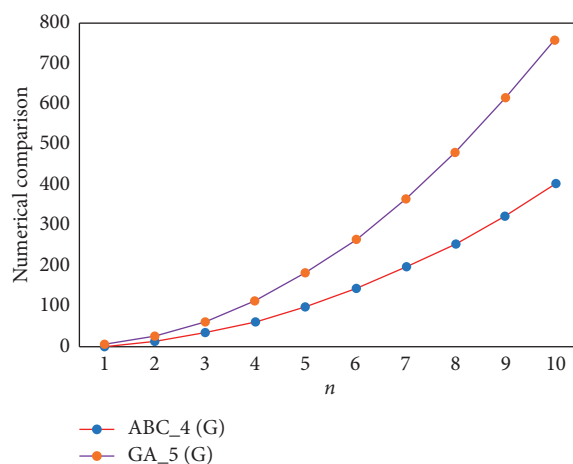


FIGURE 8: Comparison of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$.

5. Numerical and Graphical Representation

Here, we give numeric and graphic representation for the results calculated in the above section (see Tables 7 and 8).

6. Conclusion

Amylose has a significant function in the storage of plant energy. It is not easy to digest compared to amylopectin; however, it occupies less space than amylopectin due to its spiral structure. Consequently, for storage in plants, it is the preferred starch. A mixture of iodine and potassium iodide in water is light orange-brown. When added to a sample containing starch, such as the bread pictured above, the colour will change to a deep blue (see the comparison of different indices in Figures 7 and 8). In this study, we have calculated degree-dependent topological indices of amylose and blue starch-iodine. We observed that $R_{(-1/2)}$ is closely related to geometric-arithmetic, R_{-1} is closely related to atom-bond connectivity and modified atom-bond

connectivity, the second Zagreb is the first Randic index, while $R_{(1/2)}$ is approximately equal to the modified geometric-arithmetic of amylose. Similarly, other observations can take place from the graphical representations given in this paper.

Data Availability

All kinds of data and materials, used to compute the results, are provided in Section 1.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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