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

Anam Rani¹, Usman Ali²,³,*

¹ Department of Basics Sciences, Deanship of Preparatory Year King Faisal University Al Ahsa, Saudi Arabia
² Institute de Mathematiques de Jussieu-Paris Rive Gauche -Paris, France (Universite de Paris/Sorbonne Universite)
³ CASPAM, Bahauddin Zakariya University, Multan 66000, Pakistan
arani@kfu.edu.sa, uali@bzu.edu.pk

Abstract

Starch is a polymer of glucose where alpha-linkages 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 dextrins, 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 $\alpha = -\frac{1}{2}, -1, \frac{1}{2}, 1$, Atom-bond connectivity index $ABC(\Gamma)$, Geometric arithmetic index $GA(\Gamma)$, fourth Atom-bond connectivity index $ABC_4(\Gamma)$ and fifth Geometric arithmetic index $GA_5(\Gamma)$, degree-based topological indices a graph $\Gamma$ representing Polysaccharides, namely, Amylose and Blue Starch Iodine Complex. In the end, we compare these indices and depict their graphic behavior.

Keywords: Polysaccharides, Amylose, Blue Starch Iodine Complex, Zagreb index, Randić index, Atom-bond connectivity index, Geometric arithmetic index

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 is 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.

*Corresponding author
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 [2] described the M-polynomial and degree-based topological indices of graphs. The articles [7, 9] discussed the symmetric divisor deg index of graphs, first Zegrab after 30 years in changed form and topological indices of molecular structure. The authors in [10] also discussed the $\pi$ electron energy of hydrocarbons. In the recent years, Hasni et al. computed the degree based topological indices of line graph of benzene ring embedded in P-type-surface in 2D network [1]. In [11] the authors calculated the index numbers for the edge version of 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 $\Gamma$ 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 $\tilde{R}_u$. The idea of degree-based topological indices began from Wiener index, in 1945, Wiener defined them while studying alkane’s boiling point cf. [15]. The first degree-based topological index is Randić index given by Milan Randić in [12] and is described as:

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

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

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

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

$$RR_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{(\sqrt{\tilde{R}_u \tilde{R}_v})^\alpha}$$

In [8, 10] and [13], 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:

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

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

In [3], Estrada introduced and studied about the Atom-bond connectivity index (denoted as $ABC(\Gamma)$). It is defined as:

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

Geometric-arithmetic index (denoted as $GA(\Gamma)$) was given by Vukičević cf. [14] and is defined as:

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

The fourth version of the ABC index (denoted as $ABC_4(\Gamma)$) was introduced by Ghorbani in [4] and is defined as:
\[ ABC_4(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{S_u + S_v - 2} \quad (5) \]

where \( S_u = \sum_{v=N_\Gamma(u)} \tilde{\Re}_v \) 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. [5] and is defined as:

\[ GA_5(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \quad (6) \]

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 \( \alpha \)-D-glucose units, linked by \( \alpha (1 \rightarrow 4) \) 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 [6] (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:

- \( E_{1,2}(\Gamma) = \{ \tilde{\Re}_u = 1, \text{ } \tilde{\Re}_v = 2 \text{ and } u, v \in V(\Gamma) \} \)
- \( E_{1,3}(\Gamma) = \{ \tilde{\Re}_u = 1, \text{ } \tilde{\Re}_v = 3 \text{ and } u, v \in V(\Gamma) \} \)
- \( E_{2,3}(\Gamma) = \{ \tilde{\Re}_u = 2, \text{ } \tilde{\Re}_v = 3 \text{ and } u, v \in V(\Gamma) \} \)
- \( E_{3,3}(\Gamma) = \{ \tilde{\Re}_u = 3, \text{ } \tilde{\Re}_v = 3 \text{ and } u, v \in V(\Gamma) \} \)

![Figure 1: Molecular structure of Amylose](image)

| 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      | \( n \)        | \( 2n + 2 \)   | \( 5n - 2 \)   | \( 4n \)       |

Table 1: Edge partition of edges based on degree of vertices
Figure 2: (a) Graph of Amylose for n=1 (b) Graph of Amylose for n=4

**Theorem 1.** For all $n \geq 2$, the graph $\Gamma$ of Amylose, we have the following:

\begin{align*}
R_1(\Gamma) &= 74n - 6 \\
R_{\frac{1}{2}}(\Gamma) &= 29.1258n - 1.4349 \\
R_{-\frac{1}{2}}(\Gamma) &= 5.2363n + 0.3382 \\
R_{-1}(\Gamma) &= 2.4444n + 0.3334
\end{align*}

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

$$R_1(\Gamma) = \sum_{uv \in E(\Gamma)} \tilde{\mathcal{R}}_u \tilde{\mathcal{R}}_v$$

From Table I and Equation I we get

$$R_1(\Gamma) = n(1 \times 2) + (2n + 2)(1 \times 3) + (5n - 2)(2 \times 3) + 4n(3 \times 3) = 74n - 6$$

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

$$R_{\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\tilde{\mathcal{R}}_u \tilde{\mathcal{R}}_v}$$

Again, from Table I and Equation I we have

$$R_{\frac{1}{2}}(\Gamma) = n \sqrt{(1 \times 2) + (2n + 2) \sqrt{(1 \times 3) + (5n - 2) \sqrt{(2 \times 3) + 4n \sqrt{(3 \times 3)}}}} = 29.1258n - 1.4349$$

If $\alpha = -\frac{1}{2}$, then

$$R_{-\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\tilde{\mathcal{R}}_u \tilde{\mathcal{R}}_v}}$$
From Table 1 and Equation 1, it follows that

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

$$= 5.2363n + 0.3382$$

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

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

From Table 1 and Equation 1, we get

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

$$= 2.4444n + 0.3334$$

**Theorem 2.** For all $n \geq 2$, $\Gamma$ be the graph of Amylose. Then we have the following:

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

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

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

$$GA(\Gamma) = 11.5738n - 0.2276$$

**Proof.** By using Table 1 and Equation 2, we get

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

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

$$= 60n - 2$$

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

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

$$= 74n - 6$$

By using Table 1 and Equation 3, we get

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

$$= n\sqrt{\frac{1 + 2 - 2}{1 \times 2} + (2n + 2)\sqrt{\frac{1 + 3 - 2}{1 \times 3} + (5n - 2)\sqrt{\frac{2 + 3 - 2}{2 \times 3} + 4n\sqrt{\frac{3 + 3 - 2}{3 \times 3}}}}$$

$$= 8.5423n + 0.2188$$
By using Table 1 and Equation 4 we get
\[
GA(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\overline{\mathbb{R}}_u \overline{\mathbb{R}}_v}}{\overline{\mathbb{R}}_u + \overline{\mathbb{R}}_v}
\]
\[
= 2\left( n \sqrt{\frac{1 \times 2}{1 + 2}} + (2n + 2) \sqrt{\frac{1 \times 3}{1 + 3}} + (5n - 2) \frac{\sqrt{2 \times 3}}{2 + 3} + 4n \frac{\sqrt{3 \times 3}}{3 + 3} \right)
\]
\[
= 11.5738n - 0.2276
\]

In the following table, we give the edge partition centered on degree sum of end vertices for 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           | $3n - 1$    | $n - 1$     | 2           | $n - 2$     |

Table 2: Edge partition based on degree sum of end vertices of each edge

**Theorem 3.** For all $n \geq 2$, the graph $\Gamma$ of Amylose, we have

\[
ABC_4(\Gamma) = 6.4972n + 0.2874
\]

\[
GA_5(\Gamma) = 11.7142n - 0.123
\]

**Proof.** By using Table 2 and Equation 5 we get

\[
ABC_4(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}
\]
\[
= n \sqrt{\frac{2 \times 4 - 2}{2 \times 4}} + \sqrt{\frac{3 \times 6 - 2}{3 \times 6}} + (2n + 1) \sqrt{\frac{3 \times 7 - 2}{3 \times 7}} + n \sqrt{\frac{4 \times 7 - 2}{4 \times 7}} + \sqrt{\frac{6 \times 6 - 2}{6 \times 6}}
\]
\[
+ (3n - 1) \sqrt{\frac{6 \times 7 - 2}{6 \times 7}} + (n - 1) \sqrt{\frac{6 \times 8 - 2}{6 \times 8}} + (2n + 1) \sqrt{\frac{7 \times 7 - 2}{7 \times 7}} + (2n - 2) \sqrt{\frac{7 \times 8 - 2}{7 \times 8}}
\]
\[
= 6.4972n + 0.2874
\]

By using Table 2 and Equation 6 we get

\[
GA_5(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}
\]
\[
= 2\left( n \sqrt{\frac{2 \times 4}{2 + 4}} + \sqrt{\frac{3 \times 6}{3 + 6}} + (2n + 1) \sqrt{\frac{3 \times 7}{3 + 7}} + n \sqrt{\frac{4 \times 7}{4 + 7}} + \sqrt{\frac{6 \times 6}{6 + 6}} + (3n - 1) \sqrt{\frac{6 \times 7}{6 + 7}}
\]
\[
+ (n - 1) \sqrt{\frac{6 \times 8}{6 + 8}} + (2n + 1) \sqrt{\frac{7 \times 7}{7 + 7}} + (2n - 2) \sqrt{\frac{7 \times 8}{7 + 8}} \right)
\]
\[
= 11.7142n - 0.123
\]
Table 3: Numerical Comparison of $M_1(\Gamma), M_2(\Gamma), ABC(\Gamma), GA(\Gamma), R_1(\Gamma), R_{-1}(\Gamma), R_2(\Gamma),$ and $R_{-2}(\Gamma)$

| $n$ | $M_1(\Gamma)$ | $M_2(\Gamma)$ | $ABC(\Gamma)$ | $GA(\Gamma)$ | $R_1(\Gamma)$ | $R_{-1}(\Gamma)$ | $R_2(\Gamma)$ | $R_{-2}(\Gamma)$ |
|-----|---------------|---------------|---------------|---------------|---------------|-----------------|---------------|-----------------|
| 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|

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.

![Figure 3](image1.png)  ![Figure 4](image2.png)

Figure 3: (a) Comparison of $R_\alpha$ for $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$, (b) Comparison of $M_1(\Gamma), M_2(\Gamma), ABC(\Gamma)$ and $GA(\Gamma)$

4 Results for Blue Starch-Iodine Complex

The main structure for 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 $H_2O$)$_{10}HI_5$ with linear polyiodide chain. Even though this structural model was accepted. But, unfortunately, cannot shed light on the actual configuration of the polyiodide chain (see Figure 5 for Molecular structure of Blue Starch-Iodine and Figure 6 for its unit graph and the graph model corresponding to Blue Starch-Iodin 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:

$E_{1,2}(\Gamma) = \{\widetilde{\mathcal{R}}_u = 1, \widetilde{\mathcal{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}$

$E_{1,3}(\Gamma) = \{\widetilde{\mathcal{R}}_u = 1, \widetilde{\mathcal{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$

$E_{2,2}(\Gamma) = \{\widetilde{\mathcal{R}}_u = 2, \widetilde{\mathcal{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}$

$E_{2,3}(\Gamma) = \{\widetilde{\mathcal{R}}_u = 2, \widetilde{\mathcal{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$

$E_{3,3}(\Gamma) = \{\widetilde{\mathcal{R}}_u = 3, \widetilde{\mathcal{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$

Figure 4: Comparison of $ABC_4(\Gamma)$, $GA_5(\Gamma)$

Figure 5: (Molecular structure of Blue Starch-Iodine)
Figure 6: (a) Graph of Blue Starch-Iodine for n=1 (b) Graph of Blue Starch-Iodine for n=6

| 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     | $2n$        | $\sum_{i=1}^{n-1}(n+2) - 2$ | $n$        | $\sum_{i=1}^{n-1}(6n-2) + 2$ | $4n$        |

Table 5: Edge partition based on degree of vertices

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

$R_1(\Gamma) = 39n^2 - n + 12$

$R_{\frac{1}{2}}(\Gamma) = 16.429n^2 - 1.0354 + 2.8695$

$R_{-\frac{1}{2}}(\Gamma) = 3.0272n^2 + .5585n - 0.6764$

$R_{-1}(\Gamma) = 0.75n^2 + 0.6944n - 0.6667$

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

$$R_1(\Gamma) = \sum_{uv \in E(\Gamma)} \tilde{\mathcal{R}}_u \tilde{\mathcal{R}}_v$$

From Table 5 (for edge partition) and Equation 1, we get

$$R_1(\Gamma) = 2n(1 \times 2) + \left[ \sum_{i=1}^{n-1}(n+2) - 2 \right](1 \times 3) + n(2 \times 2) + \left[ \sum_{i=1}^{n-1}(6n-2) + 2 \right](2 \times 3) + 4n(3 \times 3)$$

$$= 39n^2 - n + 12$$

Now, for $\alpha = \frac{1}{2}$, we have

$$R_{\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\tilde{\mathcal{R}}_u \tilde{\mathcal{R}}_v}$$

By using Table 5 and Equation 1 after simplification, we have

$$R_{\frac{1}{2}}(\Gamma) = 2n \sqrt{(1 \times 2)} + \left[ \sum_{i=1}^{n-1}(n+2) - 2 \right] \sqrt{(1 \times 3)} + n \sqrt{(2 \times 2)} + \left[ \sum_{i=1}^{n-1}(6n-2) + 2 \right] \sqrt{(2 \times 3)} + 4n \sqrt{(3 \times 3)}$$

$$= 16.429n^2 - 1.0354 + 2.8695$$
For $\alpha = -\frac{1}{2}$, we have

$$R_{-\frac{1}{2}}(\Gamma) = \sum_{uv \in \mathcal{E}(\Gamma)} \frac{1}{\sqrt{\widetilde{\Re}_u \widetilde{\Re}_v}}$$

From Table 5 and Equation 1, it follows that

$$R_{-\frac{1}{2}}(\Gamma) = \frac{2n}{\sqrt{(1 \times 2)}} + \left[ \sum_{i=1}^{n-1} (n + 2) - 2 \right] \frac{1}{\sqrt{(1 \times 3)}} + \frac{n}{\sqrt{(2 \times 2)}} + \left[ \sum_{i=1}^{n-1} (6n - 2) + 2 \right] \frac{1}{\sqrt{(2 \times 3)}} + \frac{4n}{\sqrt{(3 \times 3)}}$$

$$= 3.0272n^2 + 0.5585n - 0.6764$$

For $\alpha = -1$, we have

$$R_{-1}(\Gamma) = \sum_{uv \in \mathcal{E}(\Gamma)} \frac{1}{\Re_u \Re_v}$$

Again by using Table 5 and Equation 1, we get

$$R_{-1}(\Gamma) = \frac{2n}{(1 \times 2)} + \left[ \sum_{i=1}^{n-1} (n + 2) - 2 \right] \frac{1}{(1 \times 3)} + \frac{n}{(2 \times 2)} + \left[ \sum_{i=1}^{n-1} (6n - 2) + 2 \right] \frac{1}{(2 \times 3)} + \frac{4n}{(3 \times 3)}$$

$$= 0.75n^2 + 0.6944n - 0.6667$$

\[ \square \]

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

$$M_1(\Gamma) = 34n^2 - 2n + 4$$

$$M_2(\Gamma) = 39n^2 - n + 12$$

$$ABC(\Gamma) = 5.0591n^2 - 0.0523n - 0.4376$$

$$GA(\Gamma) = 6.7448n^2 - 3.0868n + 0.4552$$

**Proof.** By using Table 5 and Equation 2, we get

$$M_1(\Gamma) = \sum_{uv \in \mathcal{E}(\Gamma)} (\widetilde{\Re}_u + \widetilde{\Re}_v)$$

$$= 2n(1 + 2) + \left[ \sum_{i=1}^{n-1} (n + 2) - 2 \right] (1 + 3) + n(2 + 2) + \left[ \sum_{i=1}^{n-1} (6n - 2) + 2 \right] (2 + 3) + 4n(3 + 3)$$

$$= 34n^2 - 2n + 4$$

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

$$= 2n(1 \times 2) + \left[ \sum_{i=1}^{n-1} (n + 2) - 2 \right] (1 \times 3) + n(2 \times 2) + \left[ \sum_{i=1}^{n-1} (6n - 2) + 2 \right] (2 \times 3) + 4n(3 \times 3)$$

$$= 39n^2 - n + 12$$

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By using Table 5 and Equation 3 we get

\[ \sum \text{Types of edges} \]

\[ \begin{array}{ccccccc}
\text{No. of edges} & E_{(2,3)} & E_{(2,4)} & E_{(3,5)} & E_{(3,6)} & E_{(3,7)} & E_{(4,8)} \\
\text{Frequency} & n & n & n & \sum_{i=1}^{n-1} (1) - 1 & \sum_{i=1}^{n-1} (n) - 1 & n \\
\text{Types of edges} & E_{(5,7)} & E_{(6,6)} & E_{(6,7)} & E_{(6,8)} & E_{(7,7)} & E_{(7,8)} \\
\text{No. of edges} & (5,7) & (6,6) & (6,7) & (6,8) & (7,7) & (7,8) \\
\text{Frequency} & n & \sum_{i=1}^{n-1} (1) - 1 & \sum_{i=1}^{n-1} (3n - 2) + 2 & n & \sum_{i=1}^{n-1} (2) - 2 & \sum_{i=1}^{n-1} (4n - 3) + 3 \\
\end{array} \]

Table 6: Edge partition based on degree sum of end vertices of each edge

\[ \text{Theorem 6. For all } n \geq 3, \text{ the graph } \Gamma \text{ of blue starch-iodine complex, we have} \]

\[ ABC_4(\Gamma) = 4.0798n^2 - 0.7682n + 0.04 \]

\[ GA_5(\Gamma) = 7.8987n^2 - 3.1339n + 1.1727 \]

\[ \text{Proof. By using Table 5 and Equation 5 we get} \]

\[ ABC_4(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \]

\[ = n \sqrt{\frac{2 + 3 - 2}{2 \times 3} + n \sqrt{\frac{2 + 4 - 2}{2 \times 4}} + n \sqrt{\frac{3 + 5 - 2}{3 \times 5} + (n - 2) \sqrt{\frac{3 + 6 - 2}{3 \times 6} + (n^2 - n - 1) \sqrt{\frac{3 + 7 - 2}{3 \times 7}}} + n \sqrt{\frac{4 + 8 - 2}{4 \times 8} + n \sqrt{\frac{5 + 7 - 2}{5 \times 7} + (n - 2) \sqrt{\frac{6 + 6 - 2}{6 \times 6} + (3n^2 - 5n + 4) \sqrt{\frac{6 + 7 - 2}{6 \times 7}}} + n \sqrt{\frac{6 + 8 - 2}{6 \times 8} + (2n - 4) \sqrt{\frac{7 + 7 - 2}{7 \times 7} + (4n^2 - 7n + 6) \sqrt{\frac{7 + 8 - 2}{7 \times 8}}}}}} \]

\[ = 4.0798n^2 - 0.7682n + 0.04 \]
By using Table 6 and Equation 6, we get

\[ GA_5(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)} \]

\[ = 2 \left( \frac{n \sqrt{2 \times 3}}{2 + 3} + \frac{n \sqrt{2 \times 4}}{2 + 4} + \frac{n \sqrt{3 \times 5}}{3 + 5} + (n - 2) \frac{\sqrt{3 \times 6}}{3 + 6} + (n^2 - n - 1) \frac{\sqrt{4 \times 8}}{4 + 8} + n \frac{\sqrt{5 \times 7}}{5 + 7} \right) \]

\[ + (n - 2) \frac{\sqrt{6 \times 6}}{6 + 6} + (3n^2 - 5n + 4) \frac{\sqrt{6 \times 7}}{6 + 7} + n \frac{\sqrt{6 \times 8}}{6 + 8} + (2n - 4) \frac{\sqrt{7 \times 7}}{7 + 7} + (4n^2 - 7n + 6) \frac{\sqrt{7 \times 8}}{7 + 8} \]

\[ = 7.8987n^2 - 3.1339n + 1.1727 \]

\[ \square \]

5 Numerical and Graphical Representation

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

Table 7: Numerical Comparison of \( M_1(\Gamma) \), \( M_2(\Gamma) \), \( ABC(\Gamma) \), \( GA(\Gamma) \), \( R_1(\Gamma) \), \( R_{-1}(\Gamma) \), \( R_\frac{1}{2}(\Gamma) \), and \( R_{-\frac{1}{2}}(\Gamma) \)

| \( n \) | \( M_1(\Gamma) \) | \( M_2(\Gamma) \) | \( ABC(\Gamma) \) | \( GA(\Gamma) \) | \( R_1(\Gamma) \) | \( R_{-1}(\Gamma) \) | \( R_\frac{1}{2}(\Gamma) \) | \( R_{-\frac{1}{2}}(\Gamma) \) |
|---|---|---|---|---|---|---|---|---|
| 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 |
6 Conclusion

Amylose has a significant function in the storage of plant energy. It is not easy to digest 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 color 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 $R_{-1}$ is closely related to geometric arithmetic, $R_{-1}$ is closely related to atom bond connectivity bond and modified atom bond connectivity, the second zegrab is the first Randic index, while $R_{\frac{1}{2}}$ is approximately equal to the modified geometric arithmetic of Amylose. Similarly, Other observations can take place from the graphical representations given in this paper.
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References

[1] A. Ahmad, K. Elahi, R. Hasni and M. F. Nadeem, Computing the degree based topological indices of line graph of benzene ring embedded in P-type-surface in 2D network, *J. Inf. Optim. Sci.*, 40(7)(2019), 1511-1528.

[2] E. Deutsch and S. Klavžar, M-polynomial and degree-based topological indices, *Iran. J. Math. Chem.*, 6(2)(2015), 93-102.

[3] E. Estrada and L. Torres, L. Rodríguez and I. Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.*, 37A(1998), 849-855.

[4] M. Ghorbani and M. Hosseinzadeh, Computing $ABC_4$ index of nanostar dendrimers, *Optoelectron. Adv. Mater. Rapid Commun.*, 4(2010), 1419-1422.

[5] A. Graovac, M. Ghorbani and M. Hosseinzadeh, Computing fifth geometric-arithmetic index for nanostar dendrimers, *J. Math. Nanosci.*, 1(2011), 33-42.

[6] M. Green, G. Blankenhorn and H. Hart, Which starch fraction is water-soluble, Amylose or Amylopectin? *J. Chem. Educ.*, 52(11)(1975), 729.

[7] C. Gupta, V. Lokesh, S. Shwetha and P. Ranjini, On the symmetric division deg index of graph, *Southeast Asian Bull. Math.*, 40(1)(2016), 41-51.

[8] I. Gutman and K. Das, The first zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem*, 50(1)(2004), 83-92.

[9] I. Gutman and O. Polansky, Topological indices, *Mathematical Concepts in Organic Chemistry*, Springer, 1986.

[10] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. total $\varphi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17(4)(1972), 535-538.

[11] M. F. Nadeem, S. Zafar and Z. Zahid, On the edge version of geometric-arithmetic index of nanocones, *Stud. Univ. Babes-Bolyai Chemia.*, 61(1)(2016), 273-282.

[12] M. Randić, Characterization of molecular branching, *J. Amer. Chem. Soc.*, 97(23)(1975), 6609-6615.

[13] N. Trinajstić, S. Nikolić, A. Miličević and I. Gutman, About the zagreb indices, *Kemija u industriji: Časopis kemičara i kemijskih inženjera Hrvatske*, 59(12)(2010), 577-589.

[14] D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degree of edges, *J. Math. Chem.*, 46(2009), 1369-1376.

[15] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.*, 69(1)(1947), 17-20.