Punjab University Journal of Mathematics (2022),54(1),45-53
https://doi.org/10.52280/pujm.2021.540104

Topological Invariants for the General Structure of Grape Seed Proanthocyanidins

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Received: 29 April, 2021 / Accepted: 18 January, 2022 / Published online: 27 January, 2022

Abstract.: In this paper, we formulate the degree-based topological indices such as first Zagreb index, second Zagreb index, third Zagreb index, atom bond connectivity index, geometric-arithmetic (GA) index, general sum connectivity index, hyper-Zagreb index, augmented Zagreb index, sum connectivity index and general Randic index $R_\lambda(\wp)$, for $\lambda = \left\{-1, 1, -\frac{1}{2}, \frac{1}{2}\right\}$ for grape seed Proanthocyanidins network. By using above-mentioned topological indices, this study provides us different outcomes.

AMS (MOS) Subject Classification Codes: 05C09; 05C12; 05C90; 05C92
Key Words: Vertex degree, edges, topological indices, grape seed Proanthocyanidins network.

1. INTRODUCTION

Proanthocyanidins are chemical compounds that provide the flowers of many plants or fruit their blue, purple, and red colours. They were first considered for their significance as plant colourings. However, these chemical compounds may be useful in the prevention of cancer disease. It may also be helpful in the protection of the heart diseases (heart attack) and cardiovascular system. Proanthocyanidins are a class of phenolic compounds called polyphenols and extracted from grape seeds. These belong to a subclass called flavonoids. There are many sources of food of Proanthocyanidins such as bilberries, apple peel, red

grapes, cranberries, black grapes, red wine, strawberries, red cabbage, and leaves of the bilberry bush and blueberries.

Cheminformatics is the combined study of chemistry, mathematics, and information science. In this subject, we use different mathematical methods with the help of graphs that are related to chemical structures. In this study, we use different topological invariants such as wiener index, general Randic index, atom bond connectivity index, geometric-arithmetic index, first Zagreb index, second Zagreb index, second modified Zagreb index, third Zagreb index, hyper-Zagreb index and augmented Zagreb index are used to discover the bioactivity of chemical structures [1, 2].

In 1947, the Wiener index was developed by Harry Wiener [17, 11]. The Wiener's index is computed as

$$\mathrm{W}\left(\wp\right) = \frac{1}{2} \sum_{mn \in E(\wp)} d(m,\ n)$$

where d(m, n) is the distance between m and n and d_m and d_n are the degrees of vertices m and n in $\wp$, respectively.

In 1972, Gutman and Trinajstic [8] presented Zagreb indices. In 1975, Gutman presented second Zagreb index [9, 10]. The first Zagreb index and the second Zagreb index are formulated by

$$M_1\left(\wp\right) = \sum_{mn \in E(\wp)} \left(d_m + d_n\right) \quad ,$$

$$M_2\left(\wp\right) = \sum_{mn \in E(\wp)} \left(d_m \times d_n\right)$$

In 1975, Randic index [14] was presented by Milan Randic. This index is used in cheminformatics to examine the nature of chemical compounds. The Randic index, also called the connectivity index of the graph, is computed by

$$R_{\frac{1}{2}}\left(\wp\right) = \sum_{mn \in E(\wp)} \frac{1}{\sqrt{\left(d_m \times d_n\right)}}$$

After some time, it was generalized by Bollobas and Erdos for different values of γ, where $\gamma \in \mathrm{R}$ and named as the generalized Randic index [3] and is computed by

$$R_\gamma\left(\wp\right) = \sum_{mn \in E(\wp)} \left(d_m \times d_n\right)^\gamma,\ \ for\ \ \gamma = \{\ -1,\ 1,\ -\frac{1}{2},\ \frac{1}{2}\ \}$$

A modified version of the second Zagreb index was presented in 2003 by Nikolaic [13]. The modified Zagreb index of the graph $\wp$ is formulated as

$$\mathrm{SMZ}\ \left(\wp\right) = \sum_{mn \in E(\wp)} \left(d_m \times d_n\right)^{-1}$$

In 1998, Estrada et al. [4, 5] established a new topological index, called atom bond connectivity (ABC) index and is computed by

$$\text{ABC }(\wp) = \sum_{mn \in E(\wp)} \sqrt{\frac{d_m + d_n - 2}{d_m \times d_n}}$$

In 2009, D. Vukicevic and B. Furtula projected first (GA) index in [14, 16, 18]. The first geometric-arithmetic (GA) index of a graph $\wp$ is symbolized as

$$\text{GA }(\wp) = \sum_{mn \in E(\wp)} \frac{2\sqrt{d_m \times d_n}}{d_m + d_n}$$

Furtula presented another topological invariant in 2010 and known as augmented Zagreb index [6] and is symbolized as

$$\text{AZM }(\wp) = \sum_{mn \in E(\wp)} \left(\frac{d_m \times d_n}{d_m + d_n - 2}\right)^3$$

In 2011, after the first and second Zagreb indices, the third Zagreb index was proposed in [7, 8]. This new graph invariant is formulated as

$$M_3(\wp) = \sum_{mn \in E(\wp)} |d_m - d_n|$$

A new topological index that was degree based was established, called hyper-Zagreb index [15, 10], and is calculated as

$$\text{HM }(\wp) = \sum_{mn \in E(\wp)} (d_m + \ d_n)^2$$

2. HYPOTHESIS AND LIMITATIONS OF THE DEVELOP METHOD

This work can be correlated with the chemical structure of grape seed Proanthocyanidins to understand partially its bioactivity and the physical properties by using the quantitative structure activity relationship study known as (QSARs) and quantitative structure property relationship study known as (QSPRs). There are few limitations of this work as follows:
1. It is incompletely characterized.
2. There is limited knowledge of the chemistry of Proanthocyanidins.
3. We are restricted to construct n^{th} formula to compute topological indices that can be used to correlate with the molecular compound.

3. TOPOLOGICAL INDICES FOR GRAPE SEED PROANTHOCYANIDINS NETWORK

In this section, degree based topological indices such as first Zagreb index, second Zagreb index, third Zagreb index, atom bond connectivity index, geometric-arithmetic (GA) index, general sum connectivity index, hyper-Zagreb index, augmented Zagreb index, sum connectivity index and general Randic index $R_\lambda(\wp)$, for $\lambda = \left\{-1, 1, -\frac{1}{2}, \frac{1}{2}\right\}$ for grape seed Proanthocyanidins network will be computed.

4. MAIN ADVANTAGES AND DISADVANTAGES OF THIS WORK

Proanthocyanidins, the most abundant polyphenols in human diets, have multiple health benefits. Proanthocyanidins from grape seeds are highly antioxidants. The results obtained can be correlated with the chemical structure of grape seed Proanthocyanidins to understand the main advantages, disadvantages, its bioactivities as well as physical properties.

5. METHODOLOGY

Different topological indices are used to compare the mathematical structure of the graph with the chemical structure of the compound to know their topologies. In this process the main technique used is the topological descriptor and having the following steps for computations.

1. **Graph:** Association of the graph with the chemical structure.
2. **Vertex Labelling:** Label each vertex with their degrees.
3. **Edges Partition:** Separation of edge set according to their degrees.
4. **Computations:** Calculations of degree of each vertex to get the general formula.

6. RESULTS FOR GRAPE SEED PROANTHOCYANIDINS NETWORK

There are several natural foodstuffs extracted from plants that are being explored as healthy ingredients because of their configuration in bioactive compounds. Some of those bioactive compounds, phenolic compounds, characterize one of the most stimulating groups. The variety and the high number of compounds from this group is well-known. Proanthocyanidins (PACs) [12, 19]. They can easily be found in fruits such as berries or grapes, and in some others, like cocoa, chocolate, wine, peanuts, almonds, and avocadoes. We denote the general structure of grape seed Proanthocyanidins network by GSP_n. In the grape seed Proanthocyanidin network GSP_n, the number of vertices and edges are $16n$ and $19n - 1$, respectively. We have found here three different categories of edges which are purely degree based. These edges are (2, 2), (2, 3) & (3, 3). Table-1 shows three types of edges. Grape seed Proanthocyanidin network GSP_n is displayed in Figure-1.

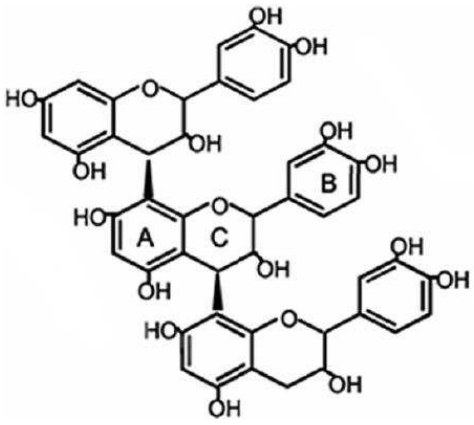

FIGURE 1. GSP_3

TABLE 1. Partition of edges of a graph GSP_3 formed by the degrees of terminating nodes of each of the edges.

$(d_m,\ d_n)\ for\ mn \in E(\wp)$	$Number\ of\ E(\wp)$
(2, 2)	*6n+2*
(2, 3)	*8n*
(3, 3)	*5n-3*

Figure 1 illustrates 3-dimensional grape seed Proanthocyanidins network. We introduce here two essential components known as nodes and edges for the graph shown in Figure 1 and symbolized by $\wp$.

Theorem 6.1:- For the grape seed Proanthocyanidins network, GSP_n, first Zagreb index can be calculated as:-

$$M_1(\wp) = 94n - 10.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP_n. By Table 1, we have

$$M_1(\wp) = \sum_{pq \in E(\wp)} (d_p + d_q)$$

$$M_1(\wp) = (6n+2)(4) + 8n(5) + (5n-3)(6) = 94n - 10.$$

Theorem 6.2:- For the grape seed Proanthocyanidins network, GSP_n, second Zagreb index can be calculated as:-

$$M_2(\wp) = 117n - 19.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP_n. By Table 1, we have

$$M_2(\wp) = \sum_{pq \in E(\wp)} (d_p \times d_q)$$

$$M_2(\wp) = (6n+2)(4) + 8n(6) + (5n-3)(9) = 117n - 19.$$

Theorem 6.3:- For the grape seed Proanthocyanidins network, GSP_n, third Zagreb index can be calculated as:-

$$M_3(\wp) = 8n.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP_n. By Table 1, we have

$$M_3(\wp) = \sum_{pq \in E(\wp)} |d_p - d_q|$$

$$M_3(\wp) = (6n+2)(0) + 8n|-1| + (5n-3)(0) = 8n.$$

Theorem 6.4:- For the grape seed Proanthocyanidins network, GSP_n, atom bond connectivity index can be calculated as:-

$$\text{ABC}(\wp) = 2n\left\{\frac{7}{\sqrt{2}} + \frac{5}{3}\right\} + \{\sqrt{2} - 2\}.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$. By Table 1, we have

$$\mathrm{ABC}(\wp) = \sum_{\mathrm{pq} \in E(\wp)} \sqrt{\frac{d_p + d_q - 2}{d_p \times d_q}}$$

$$\mathrm{ABC}(\wp) = (6n+2)\sqrt{\frac{2+2-2}{4}} + 8n\sqrt{\frac{2+3-2}{6}} + (5n-3)\sqrt{\frac{3+3-2}{9}}$$

$$= 2n\left\{\frac{7}{\sqrt{2}} + \frac{5}{3}\right\} + \{\sqrt{2} - 2\}.$$

Theorem 6.5:- For the grape seed Proanthocyanidins network, GSP$_n$, geometric-arithmetic index can be calculated as:-

$$\mathrm{GA}(\wp) = n\left\{11 + \frac{16\sqrt{6}}{5}\right\} - 1.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$. By Table 1, we have

$$\mathrm{GA}(\wp) = \sum_{\mathrm{pq} \in E(\wp)} \frac{2\sqrt{d_p \times d_q}}{d_p + d_q}$$

$$\mathrm{GA}(\wp) = (6n+2) + (8n)\frac{2\sqrt{6}}{5} + (5n-3)\frac{2\sqrt{9}}{6}$$

$$= n\left\{11 + \frac{16\sqrt{6}}{5}\right\} - 1.$$

Theorem 6.6:- For the grape seed Proanthocyanidins network, GSP$_n$, general sum connectivity index can be calculated as:-

$$\chi_k(\wp) = n\{6\left\{4^k\right\} + 8\left\{5^k\right\} + 5\{6^k\}\} + \{2\{4^k\} - 3\{6^k\}\}.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$. By Table 1, we have

$$\chi_k(\wp) = \sum_{\mathrm{pq} \in E(\wp)} [d_p + d_q]^k$$

$$\chi_k(\wp) = (6n+2)\left(4^k\right) + 8n\left(5^k\right) + (5n-3)\left(6^k\right)$$

$$= n\{6\left\{4^k\right\} + 8\left\{5^k\right\} + 5\{6^k\}\} + \{2\{4^k\} - 3\{6^k\}\}.$$

Theorem 6.7:- For the grape seed Proanthocyanidins network, GSP$_n$, sum connectivity index can be calculated as:-

$$\chi_{-\frac{1}{2}}(\wp) = n\left\{3 + \frac{8}{\sqrt{5}} + \frac{5}{\sqrt{6}}\right\} + \{1 - \frac{3}{\sqrt{6}}\}.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$. By Table 1, we have

$$\chi_{-\frac{1}{2}}(\wp) = \sum_{\mathrm{pq} \in E(\wp)} [d_p + d_q]^{-\frac{1}{2}}$$

$$\chi_{-\frac{1}{2}}(\wp) = (6n+2)\left(\frac{1}{2}\right) + (8n)\left(\frac{1}{\sqrt{5}}\right) + (5n-3)\left(\frac{1}{\sqrt{6}}\right)$$
$$= n\left\{3 + \frac{8}{\sqrt{5}} + \frac{5}{\sqrt{6}}\right\} + \{1 - \frac{3}{\sqrt{6}}\}.$$

Theorem 6.8:- For the grape seed Proanthocyanidins network, GSP$_n$, hyper-Zagreb index can be calculated as:-

$$\mathrm{HM}(\wp) = 476n - 76.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$. By Table 1, we have

$$\mathrm{HM}(\wp) = \sum_{\mathrm{pq} \in E(\wp)} [d_p + d_q]^2$$

$$\mathrm{HM}(\wp) = (6n+2)(16) + 8n(25) + (5n-3)(36) = 476n - 76.$$

Theorem 6.9:- For the grape seed Proanthocyanidins network, GSP$_n$, augmented Zagreb index can be calculated as:-

$$\mathrm{AZ}(\wp) = n\left\{\frac{10813}{64}\right\} - \left\{\frac{1163}{64}\right\}.$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$. By Table 1, we have

$$\mathrm{AZ}(\wp) = \sum_{\mathrm{pq} \in E(\wp)} \left(\frac{d_p \times d_q}{d_p + d_q - 2}\right)^3$$

$$\mathrm{AZ}(\wp) = (6n+2)\left(\frac{4}{2+2-2}\right)^3 + 8n\left(\frac{6}{2+3-2}\right)^3 + (5n-3)\left(\frac{9}{3+3-2}\right)^3$$
$$= n\left\{\frac{10813}{64}\right\} - \left\{\frac{1163}{64}\right\}.$$

Theorem 6.10:- For the grape seed Proanthocyanidins network, GSP$_n$, general Randic index can be calculated as:-

$$R_\lambda(GSP_n) = \begin{cases} \frac{61n+3}{18} & \text{for } \lambda = -1 \\ n\left[\frac{14}{3} + \frac{8}{\sqrt{6}}\right] & \text{for } \lambda = -\frac{1}{2} \\ n\left[27 + 8\sqrt{6}\right] - 5 & \text{for } \lambda = \frac{1}{2} \\ 117n - 19 & \text{for } \lambda = 1 \end{cases}$$

Proof: Suppose $\wp$ is the graph of grape seed Proanthocyanidins network GSP$_n$ of n-dimensions. Then the order and size of GSP$_n$ are defined as |V(GSP$_n$)| = $16n$ and |E(GSP$_n$)| = $19n - 1$, respectively. We know that

$$R_\lambda(\wp) = \sum_{\mathrm{pq} \in E(\wp)} (d_p \times d_q)^\lambda \text{ ----------}(1),\ for\ \lambda = \{-1,\ 1,\ -\frac{1}{2},\ \frac{1}{2}\}.$$

Case 1: For λ = -1, Randic index $R_\lambda(\wp)$ can be calculated as

$$R_{-1}(\wp) = \sum_{pq \in E(\wp)} \frac{1}{d_p \times d_q}.$$

Using Table 1 and equation (1), we get

$$R_{-1}(\wp) = (6n+2)(4)^{-1} + 8n(6)^{-1} + (5n-3)(9)^{-1}.$$

After some computations, we have

$$R_{-1}(\wp) = \frac{61n+3}{18}.$$

Case 2: For λ = - $\frac{1}{2}$, Randic index $R_\lambda(\wp)$ can be calculated as

$$R_{-\frac{1}{2}}(\wp) = \sum_{pq \in E(\wp)} \frac{1}{\sqrt{(d_p \times d_q)}}.$$

Using Table 1 and equation (1), we get

$$R_{-\frac{1}{2}}(\wp) = (6n+2)\frac{1}{\sqrt{4}} + 8n\frac{1}{\sqrt{6}} + (5n-3)\frac{1}{\sqrt{9}}.$$

After some computations, we have

$$R_{-\frac{1}{2}}(\wp) = n\left\{\frac{14}{3} + \frac{8}{\sqrt{6}}\right\}.$$

Case 3: For λ = $\frac{1}{2}$, Randic index $R_\lambda(\wp)$ can be calculated as

$$R_{\frac{1}{2}}(\wp) = \sum_{pq \in E(\wp)} \sqrt{d_p \times d_q}\,.$$

Using Table 1 and equation (1), we get

$$R_{\frac{1}{2}}(\wp) = (6n+2)\sqrt{4} + 8n\sqrt{6} + (5n-3)\sqrt{9}\,.$$

After some computations, we have

$$R_{\frac{1}{2}}(\wp) = n\left\{27 + 8\sqrt{6}\right\} - 5.$$

Case 4: For λ = 1, Randic index $R_\lambda(\wp)$ can be calculated as

$$R_1(\wp) = \sum_{pq \in E(\wp)} (d_p \times d_q)^1\,.$$

Using Table 1 and equation (1), we get

$$R_1(\wp) = (6n+2)(4) + 8n(6) + (5n-3)(9)\ .$$

After some computations, we have

$$R_1(\wp) = 117n - 19.$$

7. CONCLUSIONS

Degree based topological indices such as first Zagreb, second Zagreb, third Zagreb, atom bond connectivity, geometric arithmetic (GA), general sum connectivity, hyper Zagreb, augmented Zagreb, sum connectivity and general Randic $R_\lambda(\wp)$, for $\lambda = \left\{-1, 1, -\frac{1}{2}, \frac{1}{2}\right\}$ indices for grape seed Proanthocyanidins network are discussed to study their topologies. In the coming research papers, we would like to discuss some new graphs and chemical structures to understand their topologies, entropies, and eigenvalues.

8. ACKNOWLEDGMENTS

I would like to offer my gratitude to those who encouraged, helped, advised and guided me to get better research work. I would like to thank for their precious time and efforts.

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