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Computing topological descriptors for the molecular structure of anticancer drug

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ABSTRACT

The aim of this paper is to investigate various degree based, neighborhood based and eccentricity based topological indices by considering edge partitioning method, for the molecular structure of anticancer drug Pectin, without going to the wet lab. We have computed general Randic index, general sum connectivity index, general harmonic index, Zareb indices, atom bond connectivity, geometric arithmetic index, the 4th version of atom bond connectivity index, the 5th version of geometric arithmetic index, Sanskruti index, the 5th version of atom bond connectivity index and 4th version of the geometric arithmetic index, for the molecular graph.

1. Introduction

There are several topological indices such as degree based topological indices, distance based topological indices and counting related topological indices etc. These topological indices help to correlate certain physicochemical properties such as boiling point, melting point, stability of chemical compounds etc. In this paper, we compute a variety of topological indices for the molecular structure of Pectin. Moreover, analytically closed formulas for the indices are given which will be helpful in studying the underlying topologies.

Topological indices are numerical descriptors of different chemical graphs associated with quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) (Akhter and Imran, 2016; Bača et al., 2015; Baig et al., 2015a; Foruzanfar et al., 2017). Consider G(V, E) be a simple connected graph, in which V(G) represent a non-empty set of vertices and E(G) represent a set of edges in G. In chemical graph theory, the atoms of molecules correspond to the vertices whereas the chemical bond is reflected by the edges. The history of topological indices are traced back from 1947 by Wiener, while he was working on the boiling point of paraffin.

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Bača et al. (2015) calculated topological indices depending upon two different types of edge partitioning for the molecular structure of fullerene and carbon nanotube networks. Gao et al. (2016) studied some topological indices for the molecular structure of smart polymers. Some recent work on topological indices of chemical structures have been studied in Foruzanfar et al. (2017), Gao et al. (2017, 2018), and Zhang et al. (2017). Akhter et al. (2016) and Akhter et al. (2017) defined bounds for general sum connectivity index for graph operations and composite graphs, in Akhter et al. (2016) bounds for general sum connectivity index and general Randic′ index for cacti are stated. Nadeem (2015, 2016) focus on finding the topological indices for the molecular structure of line graph of subdivision graph. Whereas, in Baig et al. (2015b) different topological polynomials are calculated.

The general Randic index was defined by Randic (1975),

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha. \quad (1)$$

The general sum connectivity index was defined by Zhou and Trinajstić (2010),

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d_u + d_v)^\alpha. \quad (2)$$

Yan et al. (2015) gave the general version of harmonic index,

$$H_k(G) = \sum_{uv\in E(G)} \left(\frac{2}{d_u+d_v}\right)^k. \quad (3)$$

Ranjini et al. (2013) stated the redefined first, second and third Zareb indices,

$$ReZG_1(G) = \sum_{uv\in E(G)} \left(\frac{d_u+d_v}{d_u d_v}\right), \quad (4)$$
$$ReZG_2(G) = \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u+d_v}\right), \quad (5)$$
$$ReZG_3(G) = \sum_{uv\in E(G)} (d_u d_v)(d_u + d_v). \quad (6)$$

Whereas Estrada et al. (1998) presented the atomic bond connectivity index,

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}. \quad (7)$$

Furtula et al. (2010) stated geometric arithmetic index as,

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}. \quad (8)$$

The 4th version of atomic bond connectivity index is defined by Ghorbani and Hosseinzadeh (2010),

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_u S_v}}. \quad (9)$$

The 5th version of geometric arithmetic index is defined by Graovac et al. (2011),

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u+S_v}. \quad (10)$$

The sanskruti index is stated by Hosamani (2017),

$$S(G) = \sum_{uv\in E(G)} \left(\frac{S_u S_v}{S_u+S_v-2}\right)^3. \quad (11)$$

The 5th version of atomic bond connectivity index is defined by Farahani (2013),

$$ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{\varepsilon_u+\varepsilon_v-2}{\varepsilon_u \varepsilon_v}}. \quad (12)$$

The 4th version of geometric arithmetic index is defined by Ghorbani and Khaki (2010),

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u+\varepsilon_v}. \quad (13)$$

2. Motivation

Pectin is a complex mixture of polysaccharides that are present in terrestrial plants. It is a major component which helps to bind cells together. Its structure, amount and chemical composition differs within a plant overtime, in various parts of a plant and among plants. Several distinct polysaccharides have been discovered and classified within the pectin group. Pectins are divided into two major groups on the basis of their degree of esterification, they are rich in galacturonic acid and they are soluble in pure water. Homogalacturonans are linear chains of α-(1-4)-linked D-galacturonic acid (Braidwood et al., 2013; Thakur et al., 1997). Pectin is a natural bipolymer, in recent years it has gained importance by scientists and pharmacists because of its tremendous benefits in a variety of industries, health promotion and treatment. Pectin is a fiber, extracted mainly from citrus fruits. It is commercially produced as a white to light brown powder. It has several unique properties that have enabled it to be used in food industry, people use pectin to control high cholesterol and diabetes, and it is used for the delivery of variety of drugs, proteins and cells. It is also used to prevent poisoning from heavy metal, colon cancer and prostate cancer (Glinsky and Raz, 2009; Guess et al., 2003; Ji et al., 2017; Wong et al., 2011; Zhang et al., 2015). Inspired by its numerous uses in diverse fields, we have decided to calculate its topological descriptors.

3. Main results and discussion

In the present era of fast development, the field of science and technology has evolved to a great extent. At one side, we have made new discoveries and found new techniques, materials and medication then on the other side we still have a variety of new complicated unsolved research problems. By the good fortune in chemical graph theory, researchers have found a strong connection between the topology of the molecular structure and its chemical characteristics, physical behaviour and biological features. Various topological indices are employed to calculate these parameters for different chemical structures. Therefore, helping the researchers to provide theoretical ground for the production of chemical products.

In this section we calculate the topological indices for the molecular structure of Pectin. Further, we provide the closed form formulas for the defined topological descriptors. Whereas, at the end conclusion has been drawn and some future work is defined.

Let P (V, E) be the graph of pectin, it has order, $|V| = 10n + 1$ and size, $|E| = 11n$, and following different types of edges.

i. The degree of any vertex u is defined as the number of edges adjacent to it. First we partition the edges based on degree of its vertices. For this graph degree based types of edges are $(1, 3), (2, 3)$ and $(3, 3)$ with count $3n + 2, 4n - 2$ and $4n$ respectively.
ii. Similarly, the neighborhood degree of any vertex u is defined as the sum of degree of vertices adjacent to it. Next we partition the edges based on neighborhood degree of its vertices. Based on neighborhood degree the types of edges for this graph are $(3, 6), (3, 7), (6, 7), (6, 8), (7, 8), (6, 6)$ and $(7, 7)$ with count $n + 1, 2n + 1$, $2n, 2n - 2$, $n - 1, n + 1$ and $2n$ respectively.
iii. Whereas, the eccentricity of any vertex u is defined as the largest distance between u and any other vertex v. Now, when we try to partition the types of edges depending upon eccentricity there is a need to distinguish n as even and odd:

- For $n \geq 2$; *even* $(5n - i, 5n - i - 1)$; i=0, 1, 2, ..., $a - 1$; with count sequence 2, 7, 7 , 4, 2 respectively, same pattern of sequence will repeat, as we increase n. Where, a will be 5 for $n = 2$, 10 for $n = 4$, 15 for $n = 6$ and so on.

- For $n \geq 3$; odd $(5n - i, 5n - i - 1)$; i=0, 1, 2, ..., $b - 4$; with count 2,7, 7,4, 2 respectively, same sequence of count will repeat, as we increase n. The last three $(b + 2,\ b + 1), (b + 1, b), (b, b)$ have fix count 2,7,2 respectively. Where, b will be 8 for $n = 3$, 13 for $n = 5$, 18 for $n = 7$ and so on.

iv. For the line graph of k-subdivided graph, where $k \geq 2$. Vertex degree based types of edges are $(1,2), (2,2)$, $(2,3)$ and $(3,3)$ with count $3n + 2, 11kn - 16n - 3, 15n$ and $15n$ respectively.

v. Similarly, for the line graph of k-subdivided graph, where $k \geq 4$. Neighborhood vertex degree based types of edges are $(2,3), (3,4), (4,4), (4,5), (5,8)$ and $(8,8)$ with count $3n + 2, 3n + 2$, $11kn - 34n - 5, 15n$, $15n$ and $15n$ respectively.

Theorem 3.1: The general version of Randic index, sum connectivity index and harmonic index for the molecular structure of pectin are,

$i). R_\alpha(P) = (2^{\alpha+2}.3^\alpha + 3^{\alpha+1} + 4.3^{2\alpha})n + 2.3^\alpha - 2^{\alpha+1}.3^\alpha,$
$ii). \chi_\alpha(P) = (2^{\alpha+2}.3^\alpha + 3.2^{2\alpha} + 4.5^\alpha)n + 2^{2\alpha+1} - 2.5^\alpha,$
$iii). H_k(P) = (3.2^{-k} + 2^{2+k}.5^{-k} + 4.3^{-k})n + 2^{1-k} - 2^{1+k}.5^{-k}.$

Proof:

i). By using the above information and inserting the values in formula 1, we get

$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$
$= (3n + 2)(1.3)^\alpha + (4n - 2)(2.3)^\alpha + (4n)(3.3)^\alpha,$
$= (3n + 2)(3)^\alpha + (4n - 2)(6)^\alpha + (4n)(9)^\alpha,$
$= (2^{\alpha+2}.3^\alpha + 3^{\alpha+1} + 4.3^{2\alpha})n + 2.3^\alpha - 2^{\alpha+1}.3^\alpha.$

ii). Similarly, by using the above information and inserting the values in formula 2, we get

$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha,$
$= (3n + 2)(1 + 3)^\alpha + (4n - 2)(2 + 3)^\alpha + (4n)(3 + 3)^\alpha,$
$= (3n + 2)(4)^\alpha + (4n - 2)(5)^\alpha + (4n)(6)^\alpha,$
$= (2^{\alpha+2}.3^\alpha + 3.2^{2\alpha} + 4.5^\alpha)n + 2^{2\alpha+1} - 2.5^\alpha.$

iii). Again, by using the above information and inserting the values in formula 3, we get

$\mathrm{H_k(G)} = \sum_{\mathrm{uv \in E(G)}} \left(\frac{2}{\mathrm{d_u + d_v}}\right)^{\mathrm{k}},$
$= (3\mathrm{n} + 2)\left(\frac{2}{1+3}\right)^{\mathrm{k}} + (4\mathrm{n} - 2)\left(\frac{2}{2+3}\right)^{\mathrm{k}} + (4\mathrm{n})\left(\frac{2}{3+3}\right)^{\mathrm{k}},$
$= (3\mathrm{n} + 2)\left(\frac{1}{2}\right)^{\mathrm{k}} + (4\mathrm{n} - 2)\left(\frac{2}{5}\right)^{\mathrm{k}} + (4\mathrm{n})\left(\frac{1}{3}\right)^{\mathrm{k}},$
$= (3.2^{-\mathrm{k}} + 2^{2+\mathrm{k}}.5^{-\mathrm{k}} + 4.3^{-\mathrm{k}})\mathrm{n} + 2^{1-\mathrm{k}} - 2^{1+\mathrm{k}}.5^{-\mathrm{k}}.$

Theorem 3.2: The redefined first, second and third Zareb indices for the molecular structure of pectin are,

$i). ReZG_1(P) = 10n + 1,$
$ii). ReZG_2(P) = \left(\frac{261}{20}\right)n - \frac{9}{10},$
$iii). ReZG_3(P) = 372n - 36.$

Proof:

i) By inserting the values in formula 4, we get

$ReZG_1(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{d_u d_v}\right),$
$= (3n + 2)\left(\frac{1+3}{1.3}\right) + (4n - 2)\left(\frac{2+3}{2.3}\right) + (4n)\left(\frac{3+3}{3.3}\right),$
$= 10n + 1.$

ii) Similarly, inserting the values in formula 5, we get

$ReZG_2(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v}\right),$
$= (3n + 2)\left(\frac{1.3}{1+3}\right) + (4n - 2)\left(\frac{2.3}{2+3}\right) + (4n)\left(\frac{3.3}{3+3}\right),$
$= \left(\frac{261}{20}\right)n - \frac{9}{10}.$

iii) Again, inserting the values in formula 6, we get

$ReZG_3(G) = \sum_{uv \in E(G)} (d_u d_v)(d_u + d_v),$
$= (3n + 2)(1.3)(1 + 3) + (4n - 2)(2.3)(2 + 3) + (4n)(3.3)(3 + 3),$
$= 372n - 36.$

Theorem 3.3: The atomic bond connectivity index and geometric arithmetic index for the molecular structure of pectin are as follows,

$i). ABC(P) = \left(\sqrt{6} + 2\sqrt{2} + \frac{8}{3}\right)n + 2\sqrt{\frac{2}{3}} - \sqrt{2},$
$ii). GA(P) = \left(\frac{3\sqrt{3}}{2} + \frac{8\sqrt{6}}{5} + 4\right)n + \sqrt{3} - \frac{4\sqrt{6}}{5}.$

Proof:

i) By inserting the values in formula 7, we get

$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$
$= (3n + 2)\sqrt{\frac{1+3-2}{1.3}} + (4n - 2)\sqrt{\frac{2+3-2}{2.3}} + (4n)\sqrt{\frac{3+3-2}{3.3}},$
$= (3n + 2)\sqrt{\frac{2}{3}} + (4n - 2)\sqrt{\frac{1}{2}} + (4n)\frac{2}{3},$
$= \left(\sqrt{6} + 2\sqrt{2} + \frac{8}{3}\right)n + 2\sqrt{\frac{2}{3}} - \sqrt{2}.$

ii) Similarly, inserting the values in formula 8, we get

$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$
$= (3n + 2)\frac{2\sqrt{1.3}1+3}{+}(4n - 2)\frac{2\sqrt{2.3}2+3}{+}(4n)\frac{2\sqrt{3.3}3+3}{,}$
$= (3n + 2)\frac{\sqrt{32}}{+}(4n - 2)\frac{2\sqrt{65}}{+}4n,$
$= \left(\frac{3\sqrt{3}}{2} + \frac{8\sqrt{6}}{5} + 4\right)n + \sqrt{3} - \frac{4\sqrt{6}}{5}.$

Theorem 3.4: The 4^{th} version of atomic bond connectivity index, 5th version of geometric arithmetic index and sanskruti index for the molecular structure of pectin are defined as,

$i)\ ABC_4(P) = \left(1 + \frac{1}{3}\sqrt{\frac{7}{2}} + \frac{\sqrt{10}}{6} + \frac{1}{2}\sqrt{\frac{13}{14}} + 2\sqrt{\frac{11}{42}} + 4\sqrt{\frac{2}{21}}\right)n$
$-1 + \frac{1}{3}\sqrt{\frac{7}{2}} + \frac{\sqrt{10}}{6} - \frac{1}{2}\sqrt{\frac{13}{14}} + \frac{4\sqrt{3}}{7} + 2\sqrt{\frac{2}{21}}$
$ii)\ GA_5(P) = \left(3 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{21}}{5} + \frac{8\sqrt{3}}{7} + \frac{4\sqrt{14}}{15} + \frac{4\sqrt{42}}{13}\right)n$

$+1+\frac{2\sqrt{2}}{3}+\frac{2\sqrt{21}}{5}-\frac{8\sqrt{3}}{7}-\frac{4\sqrt{14}}{15}$,
$iii)\ S(P)=555.2637988n-126.18765.$

Proof:

i) By using the above information and inserting the values in formula 9, we get

$$ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{s_u+s_v-2}{s_u s_v}},$$
$$=(n+1)\sqrt{\frac{7}{18}}+(2n+1)\sqrt{\frac{8}{21}}+(2n)\sqrt{\frac{11}{42}}+(2n-2)\sqrt{\frac{12}{48}}$$
$$+(n-1)\sqrt{\frac{13}{56}}+(2n)\sqrt{\frac{12}{49}}+(n+1)\sqrt{\frac{10}{36}},$$
$$=\left(1+\frac{1}{3}\sqrt{\frac{7}{2}}+\frac{\sqrt{10}}{6}+\frac{1}{2}\sqrt{\frac{13}{14}}+2\sqrt{\frac{11}{42}}+4\sqrt{\frac{2}{21}}\right)n$$
$$-1+\frac{1}{3}\sqrt{\frac{7}{2}}+\frac{\sqrt{10}}{6}-\frac{1}{2}\sqrt{\frac{13}{14}}+\frac{4\sqrt{3}}{7}+2\sqrt{\frac{2}{21}},$$
$$=4.1755014n+1.2758005.$$

ii) and iii) can be proved in a similar way by using formula 10 and 11 respectively.

Theorem 3.5: The 5th version of atomic bond connectivity index and 4th version of geometric arithmetic index are defined as follows,

Forevenn;

$$i).\ ABC_5(P)=2\left(\sum_i\sqrt{\frac{10n-2i-3}{(5n-i)(5n-i-1)}}+\sum_j\sqrt{\frac{10n-2j-3}{(5n-j)(5n-j-1)}}\right)$$
$$+7\left(\sum_p\sqrt{\frac{10n-2p-3}{(5n-p)(5n-p-1)}}+\sum_q\sqrt{\frac{10n-2q-3}{(5n-q)(5n-q-1)}}\right)$$
$$+4\sum_k\sqrt{\frac{10n-2k-3}{(5n-k)(5n-k-1)}},$$
$$ii).\ GA_4(P)=4\left(\sum_i\frac{\sqrt{(5n-i)(5n-i-1)}}{10n-2i-1}+\sum_j\frac{\sqrt{(5n-j)(5n-j-1)}}{10n-2j-1}\right)$$
$$+14\left(\sum_p\frac{\sqrt{(5n-p)(5n-p-1)}}{10n-2p-1}+\sum_q\frac{\sqrt{(5n-q)(5n-q-1)}}{10n-2q-1}\right)$$
$$+8\sum_k\frac{\sqrt{(5n-k)(5n-k-1)}}{10n-2k-1},$$
$i=0,5,10,\dots,a-5; j=4,9,14,\dots,a-1;$
$p=1,6,11,\dots,a-4; q=2,7,12,\dots,a-3;$
$k=3,8,13,\dots,a-2; a=5,10,15,\dots,$
Foroddn;

$$iii).\ ABC_5(P)=2(\sum_i\sqrt{\frac{10n-2i-3}{(5n-i)(5n-i-1)}}+$$
$$\sum_j\sqrt{\frac{10n-2j-3}{(5n-j)(5n-j-1)}}$$
$$+\sqrt{\frac{2b+1}{(b+1)(b+2)}}+\frac{\sqrt{2b-2}}{b})$$
$$+7(\sum_p\sqrt{\frac{10n-2p-3}{(5n-p)(5n-p-1)}}+\sum_q\sqrt{\frac{10n-2q-3}{(5n-q)(5n-q-1)}}$$
$$+\sqrt{\frac{2b-1}{b(b+1)}})+4\sum_k\sqrt{\frac{10n-2k-3}{(5n-k)(5n-k-1)}},$$
$$iv).\ GA_4(P)=2+4(\sum_i\frac{\sqrt{(5n-i)(5n-i-1)}}{10n-2i-1}+$$
$$\sum_j\frac{\sqrt{(5n-j)(5n-j-1)}}{10n-2j-1}$$
$$+\frac{\sqrt{(b+2)(b+1)}}{2b+3})+14(\sum_p\frac{\sqrt{(5n-p)(5n-p-1)}}{10n-2p-1}$$
$$+\sum_q\frac{\sqrt{(5n-q)(5n-q-1)}}{10n-2q-1}+\frac{\sqrt{b(b+1)}}{2b+1})$$
$$+8\sum_k\frac{\sqrt{(5n-k)(5n-k-1)}}{10n-2k-1},$$
$i=0,5,10,\dots,b-8; j=4,9,14,\dots,b-4;$
$p=1,6,11,\dots,b-7; q=2,7,12,\dots,b-6;$
$k=3,8,13,\dots,b-5; a=8,13,18,\dots.$

Proof:

i) By using the above information for *even n* and inserting the values in formula 12, we get

$$ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{\varepsilon_u+\varepsilon_v-2}{\varepsilon_u\varepsilon_v}},$$
$$=2\sum_i\sqrt{\frac{10n-i-(i+1)-2}{(5n-i)(5n-(i+1))}}+7\sum_p\sqrt{\frac{10n-p-(p+1)-2}{(5n-p)(5n-(p+1))}}$$
$$+7\sum_q\sqrt{\frac{10n-q-(q+1)-2}{(5n-q)(5n-(q+1))}}+4\sum_k\sqrt{\frac{10n-k-(k+1)-2}{(5n-k)(5n-(k+1))}}$$
$$+2\sum_j\sqrt{\frac{10n-j-(j+1)-2}{(5n-j)(5n-(j+1))}},$$
$$=2\left(\sum_i\sqrt{\frac{10n-2i-3}{(5n-i)(5n-i-1)}}+\sum_j\sqrt{\frac{10n-2j-3}{(5n-j)(5n-j-1)}}\right)$$
$$+7\left(\sum_p\sqrt{\frac{10n-2p-3}{(5n-p)(5n-p-1)}}+\sum_q\sqrt{\frac{10n-2q-3}{(5n-q)(5n-q-1)}}\right)$$
$$+4\sum_k\sqrt{\frac{10n-2k-3}{(5n-k)(5n-k-1)}},$$
$i=0,5,10,\dots,a-5; j=4,9,14,\dots,a-1;$
$p=1,6,11,\dots,a-4; q=2,7,12,\dots,a-3;$
$k=3,8,13,\dots,a-2; a=5,10,15,\dots,$

ii) Can be proved in a similar way by using formula 13.
iii) By using the above information for *odd n* and inserting the values in formula 12, we get

$$ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{\varepsilon_u+\varepsilon_v-2}{\varepsilon_u\varepsilon_v}},$$
$$=2\sum_i\sqrt{\frac{10n-i-(i+1)-2}{(5n-i)(5n-(i+1))}}+7\sum_p\sqrt{\frac{10n-p-(p+1)-2}{(5n-p)(5n-(p+1))}}$$
$$+7\sum_q\sqrt{\frac{10n-q-(q+1)-2}{(5n-q)(5n-(q+1))}}+4\sum_k\sqrt{\frac{10n-k-(k+1)-2}{(5n-k)(5n-(k+1))}}$$
$$+2\sum_j\sqrt{\frac{10n-j-(j+1)-2}{(5n-j)(5n-(j+1))}}+2\sqrt{\frac{b+2+b+1-2}{(b+2)(b+1)}}$$
$$+7\sqrt{\frac{b+1+b}{(b+1)(b)}}+2\sqrt{\frac{b+b-2}{(b)(b)}},$$
$$=2(\sum_i\sqrt{\frac{10n-2i-3}{(5n-i)(5n-i-1)}}+\sum_j\sqrt{\frac{10n-2j-3}{(5n-j)(5n-j-1)}}$$
$$+\sqrt{\frac{2b+1}{(b+1)(b+2)}}+\frac{\sqrt{2b-2}}{b})$$
$$+7(\sum_p\sqrt{\frac{10n-2p-3}{(5n-p)(5n-p-1)}}+\sum_q\sqrt{\frac{10n-2q-3}{(5n-q)(5n-q-1)}}$$
$$+\sqrt{\frac{2b-1}{b(b+1)}})+4\sum_k\sqrt{\frac{10n-2k-3}{(5n-k)(5n-k-1)}},$$
$i=0,5,10,\dots,b-8;\ j=4,9,14,\dots,b-4;$
$p=1,6,11,\dots,b-7;\ q=2,7,12,\dots,b-6;$
$k=3,8,13,\dots,b-5;\ a=8,13,18,\dots.$

iv) Can be proved in a similar way by using formula 13.

Theorem 3.6: Let G' be the line graph of k-subdivided pectin graph, where $k\geq 2$. The atom bond connectivity index and geometric arithmetic index for G' are,

$i)\ ABC(G')=\frac{11kn+2n-1}{\sqrt{2}}+10n,$
$ii)\ GA(G')=\left(\frac{4\sqrt{2}}{3}+2\sqrt{2}+6\sqrt{6}-1+11k\right)n-3.$

Proof:

i) By using the information provided above then inserting the values in formula 7, we get

$ABC(G') = \sum_{uv\in E(G')} \sqrt{\frac{d_u+d_v-2}{d_u d_v}},$
$= (3n+2)\sqrt{\frac{1+2-2}{1.2}} + (11kn-16n-3)\sqrt{\frac{2+2-2}{2.2}}$
$+15n\sqrt{\frac{2+3-2}{2.3}} + 15n\sqrt{\frac{3+3-2}{3.3}},$
$= (3n+2)\sqrt{\frac{1}{2}} + (11kn-16n-3)\sqrt{\frac{1}{2}} + 15n\sqrt{\frac{1}{2}} + 15n\sqrt{\frac{4}{9}},$
$= \frac{11kn+2n-1}{\sqrt{2}} + 10n.$

ii) By using the information provided above then inserting the values in formula 8, we get

$GA(G') = \sum_{uv\in E(G')} \frac{2\sqrt{d_u d_v}}{d_u+d_v},$
$= (3n+2)\frac{2\sqrt{1.2}}{1+2} + (11kn-16n-3)\frac{2\sqrt{2.2}}{2+2}$
$+(15n)\frac{2\sqrt{2.3}}{2+3} + (15n)\frac{2\sqrt{3.3}}{3+3},$
$= (3n+2)\frac{2\sqrt{2}}{3} + (11kn-16n-3)\frac{4}{4} + (30n)\frac{\sqrt{6}}{5} + (30n)\frac{3}{6},$
$= \left(\frac{4\sqrt{2}}{3} + 2\sqrt{2} + 6\sqrt{6} - 1 + 11k\right)n - 3.$

Theorem 3.7: Let G' be the line graph of k-subdivided pectin graph, where $k \geq 4$. The fourth version of atom bond connectivity index and fifth version of geometric arithmetic index for G' are,

i) $ABC_4(G') = (3n+2)\left(\sqrt{\frac{1}{2}} + \sqrt{\frac{5}{12}}\right) + (11kn-34n-$
$5)\sqrt{\frac{3}{8}}$
$+15n\left(\sqrt{\frac{7}{20}} + \sqrt{\frac{11}{40}} + \sqrt{\frac{7}{32}}\right),$
ii) $GA_5(G') = (6n+4)\left(\frac{\sqrt{6}}{5} + \frac{\sqrt{12}}{7}\right) + 30n\left(\frac{\sqrt{20}}{9} + \frac{\sqrt{40}}{13}\right)$
$+11kn - 4n - 5.$

Proof:

i) By using the information provided above then inserting the values in formula 9, we get

$ABC_4(G') = \sum_{uv\in E(G')} \sqrt{\frac{S_u+S_v-2}{S_u S_v}},$
$= (3n+2)\sqrt{\frac{2+3-2}{2.3}} + (3n+2)\sqrt{\frac{3+4-2}{3.4}}$
$+(11kn-34n-5)\sqrt{\frac{4+4-2}{4.4}} + 15n\sqrt{\frac{4+5-2}{4.5}}$
$+15n\sqrt{\frac{5+8-2}{5.8}} + 15n\sqrt{\frac{8+8-2}{8.8}},$
$= (3n+2)\sqrt{\frac{1}{2}} + (3n+2)\sqrt{\frac{5}{12}} + (11kn-34n-5)\sqrt{\frac{3}{8}}$
$+15n\sqrt{\frac{7}{20}} + 15n\sqrt{\frac{11}{40}} + 15n\sqrt{\frac{14}{64}},$
$= (3n+2)\left(\sqrt{\frac{1}{2}} + \sqrt{\frac{5}{12}}\right) + (11kn-34n-5)\sqrt{\frac{3}{8}}$
$+15n\left(\sqrt{\frac{7}{20}} + \sqrt{\frac{11}{40}} + \sqrt{\frac{7}{32}}\right).$

ii) By using the information provided above then inserting the values in formula 10, we get

$GA_5(G') = \sum_{uv\in E(G')} \frac{2\sqrt{S_u S_v}}{S_u+S_v},$
$= (3n+2)\frac{2\sqrt{2.3}}{2+3} + (3n+2)\frac{2\sqrt{3.4}}{3+4} + (11kn-34n-5)\frac{2\sqrt{4.4}}{4+4}$
$+(15n)\frac{2\sqrt{4.5}}{4+5} + (15n)\frac{2\sqrt{5.8}}{5+8} + (15n)\frac{2\sqrt{8.8}}{8+8},$
$= (3n+2)\frac{2\sqrt{6}}{5} + (3n+2)\frac{2\sqrt{12}}{7} + (11kn-34n-5)\frac{8}{8}$
$+(30n)\frac{\sqrt{20}}{9} + (30n)\frac{\sqrt{40}}{13} + (30n)\frac{16}{16},$
$= (6n+4)\left(\frac{\sqrt{6}}{5} + \frac{\sqrt{12}}{7}\right) + 30n\left(\frac{\sqrt{20}}{9} + \frac{\sqrt{40}}{13}\right)$
$+11kn - 4n - 5.$

4. Conclusion

The objective of this paper was to define the closed formulas, for a variety of topological indices for molecular structure of Pectin. We also computed certain indices for the line graph of k-subdivided Pectin graph. Our results are new because there is no study conducted to find such indices for Pectin. It has promising pharmaceutical uses. In future, some additional structures of anticancer drugs can be studied.

Compliance with ethical standards

Conflict of interest

The authors declare that they have no conflict of interest.

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