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Pharmacological Characteristics Analysis of Two Molecular Structures

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Abstract

Each year a large number of new diseases were found worldwide, which requires the development of new drugs to cure these diseases. In this process, researchers need to do a lot of work to test the effectiveness of new drugs and side effects. Due to the intrinsic connection between the characteristics of compound and its molecular structure, methods of pharmaceutical theory are widely used in the analysis of the features of the drug. By calculating the chemical indices of drug molecular structure, scientists could learn the chemistry and pharmacy characteristics of the corresponding drugs. In this paper, from the theoretical perspective, we state the following conclusions: (1) the exact expression of generalized degree distance for starlike tree is determined; (2) the eccentricity related indices of hetrofunctional dendrimer are discussed. The results obtained have broad application prospects in the pharmaceutical sciences.

Keywords: Theoretical pharmacy, molecular graph, topological index, dendrimer
AMS 2010 codes: 05C10.

1 Introduction

It's revealed by drug testing from the early research that the physico-chemical and pharmacological properties of drugs are closely related to their molecular structures. It raised much attention from the theoretical researchers, and until now, many topological indices are defined as useful as numerical parameters of drug structures which play an important role on understanding the properties of drugs.

In theoretical pharmacy model, a molecular structure of each drug is denoted as a molecular graph G (each atom is expressed as a vertex and each chemical bound is represented as an edge), then a topological index

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can be regarded as a score function $f : G \to \mathbb{R}^+$ which maps each molecular graph to a read positive number. In the past four decades, many indices are introduced by scholars from the engineering application prospects, such as Zagreb index, Wiener index, sum connectivity index, Gutman index and harmonic index which reflect several structural characteristics of molecules and drugs. There were many contributions to report these degree-based and distance-based indices of special molecular structures (See Farahani et al. [1], Jamil et al. [2], Gao et al. [3–7] and Gao and Wang [8–10] for more details). The notation and terminology that were used but undefined in this paper can be found in [11].

Now, we present some important indices which will be computed in the next section. The Shultz polynomial is denoted as

$$Sc(G,x) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))x^{d(u,v)}.$$

The additively weighted Harary index (also called, reciprocal degree distance) is defined as

$$H_A(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)+d(v)}{d(u,v)}.$$

As the extension, the generalized degree distance is denoted as

$$H_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))d^\lambda(u,v).$$

And, the corresponding polynomial can be stated as

$$H_\lambda(G,x) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))x^{d^\lambda(u,v)}.$$

Some results on above indices and polynomials can refer to Alizadeh et al. [12], Sedlar [13], Pourfaraj and Ghorbani [14], Pattabiraman and Vijayaragavan [15], and Hamzeh et al. [16] and [17].

Let $d(v)$ be the degree of vertex v, and $ec(v)$ be the eccentricity of vertex v which is denoted as the largest distance between v and any other vertex in molecular graph G. The first atom-bond connectivity index (ABC index) is defined by Estrada et al. [18] which is stated as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.$$

Then, the eccentricity version atom bond connectivity index (called the fifth ABC index) is denoted as

$$ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}.$$

The first geometric-arithmetic index (GA index) introduced by Vukičević and Furtula [19] which can be formulated as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}.$$

Several contributions on geometric-arithmetic index can be found in Zhou et al. [20], Rodríguez and Sigarreta [21], [22] and [23], Husin et al. [24], Bahrami and Alaeiyan [?], Sigarreta [26], Divnic et al. [27], Das et al. [28], Mahmiani et al. [29], Fath-Tabar et al. [30] and [31], Das et al. [32], Gutman and Furtula [33], Furtula and Gutman [34], and Shabani et al. [35]. The the eccentricity version geometric-arithmetic index (called the fourth GA index) is defined by Lee et al. [36] which can be expressed as

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)}.$$

Furthermore, the first and the second multiplicative version of eccentricity index are described as

$$\Pi_1^*(G) = \Pi_{uv\in E(G)}(ec(u)+ec(v))$$

and

$$\Pi_2^*(G) = \Pi_{uv\in E(G)}(ec(u)ec(v)),$$

respectively. Moreover, as related polynomials, the fourth and sixth Zagreb polynomials are defined as

$$Zg_4(G,x) = \sum_{uv\in E(G)} x^{ec(u)+ec(v)}$$

and

$$Zg_6(G,x) = \sum_{uv\in E(G)} x^{ec(u)ec(v)},$$

respectively.

Although there have been several works in topological indices of material structures, the research on topological indices for certain special drug structures is still largely limited. Furthermore, as a widespread and critical drug structure, dendrimer and starlike molecular graphs are widely used in medical science and frequently appears in new drug structures (see Kobeissi and Mollard [37], Omidi and Tajbakhsh [38], Omidi and Vatandoost [39], Betancur et al. [40] and Farooq et al. [41] for more details). It inspires us to obtain the exact expressions of some special topological indices for important classes of starlike molecular graphs and dendrimer.

The main aim of this paper is to study the generalized degree distance of starlike tree and eccentricity related indices of hetrofunctional dendrimer.

2 Main results and proofs

The purpose of this section is to present our main results and detail proofs.

2.1 Indices study of starlike tree

Let $D(G) = (d_1, d_2, \cdots, d_n)$ be the degree sequence of the graph G with $d_1 \geq d_2 \geq \cdots d_n$, where d_i denotes the degree of the i-th vertex in G. Moreover, $D(G) = (d_1^{a_1}, d_2^{a_2}, \cdots, d_t^{a_t})$ implies that G has a_i vertices with degree d_i for $i \in \{1,2,\cdots,t\}$.

A double star $S_{p,q}$ (the detailed structure can refer to Figure 1(a)) is a tree which is yielded from $K_{1,p}$ and $K_{1,q-1}$ by identifying a pendent vertex of $K_{1,p}$ with the center of $K_{1,q-1}$, where $1 < p \leq q$. Hence, for a double star $S_{p,q}$ with order n, we get $p+q=n$ and $p \leq \lfloor \frac{n}{2} \rfloor$. Furthermore, if $p = \lfloor \frac{n}{2} \rfloor$ and $q = \lceil \frac{n}{2} \rceil$, then $S_{p,q}$ is called a balanced double star.

Let $(c_1, c_2, \cdots, c_d)$ be a partition of order n. The starlike tree can be constructed using the following method:
(i) Let $S_1, S_2, \cdots, S_d$ be the stars and $v_1, v_2, \cdots, v_d$ be their center vertices. Set $|E(S_1)| = c_1 - 1, |E(S_2)| = c_2 - 1, \cdots, |E(S_d)| = c_d - 1$;
(ii) Add a vertex v_0 and then adjacent to the center vertices $v_1, v_2, \cdots, v_d$ of $S_1, S_2, \cdots, S_d$ respectively.

In this way, we can deduce a tree T with diameter at most 4, and $d_T(v_1) = c_1$, $d_T(v_2) = c_2$, $\cdots$, $d_T(v_d) = c_d$ respectively. Moreover, we infer $|V(T)| = n+1$, $E(T) = \sum_{i=1}^{d} c_i = n$. We denote this molecular structure as $S(c_1, c_2, \cdots, c_d)$ shown in Figure 1(b). Now, our main result in this part is stated as follows.

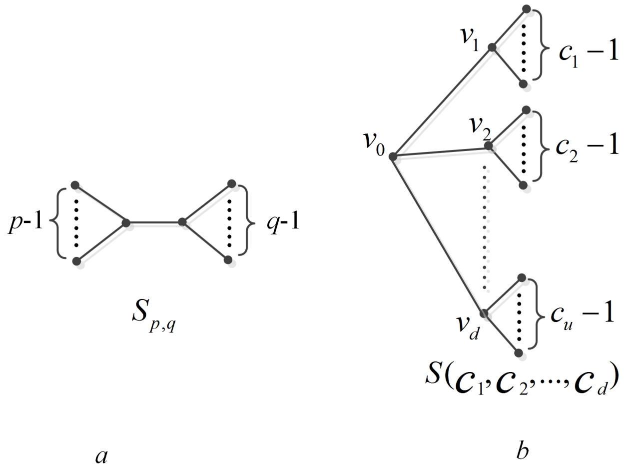

Fig. 1 Two classes of starlike tree

Theorem 1. *Let $S(c_1,c_2,\cdots,c_d)$ be a starlike tree described above. Then, we have*

$$\begin{aligned} &H_\lambda(S(c_1,c_2,\cdots,c_d)) \\ =& \sum_{i=1}^{d}(c_i^2+c_i)+d^2-d+(\sum_{i=1}^{d}(2\binom{c_i-1}{2}+(d-1)c_i)+(d+1)(n-d))\cdot 2^\lambda \\ &+(\sum_{i=1}^{d}(c_i+1)\sum_{i=1}^{d}(c_i-1)-\sum_{i=1}^{d}(c_i^2-1))\cdot 3^\lambda+2(\binom{n-d}{2}-\sum_{i=1}^{d}\binom{c_i-1}{2})\cdot 4^\lambda. \end{aligned}$$

Proof. For any pairs of vertices $(x,y)\subseteq V(S(c_1,c_2,\cdots,c_d))$, we get $d(x,y)\leq 4$. Thus, we have $d(x,y)=k$ where $k\in\{1,2,3,4\}$. The vertex set of $S(c_1,c_2,\cdots,c_d)$ can be divided into three classes: (1) the center v_0; (2) $v_1,\cdots,v_d$; (3) the leaves $w_1,w_2,\cdots,w_{n-d}$. The following discussion can be divided into four parts.

- Since $|E(S(c_1,c_2,\cdots,c_d))|=n$, there are n pairs with $d(x,y)=1$, and the total contribution of this part to generalized degree distance is

$$\sum_{i=1}^{d}(c_i+1)(c_i-1)+\sum_{i=1}^{d}(c_i+d)=\sum_{i=1}^{d}(c_i^2+c_i)+d^2-d.$$

- Vertices x and y which in pairs $(x,y)=(v_0,w_i)$, (v_i,v_j) or (w_i,w_j) satisfy $d(x,y)=2$. The total contribution of this part to generalized degree distance is

$$(\sum_{i=1}^{d}(2\binom{c_i-1}{2}+(d-1)c_i)+(d+1)(n-d))\cdot 2^\lambda.$$

- We get $d(v_i,w_j)=3$ where $i\neq j$, and the total contribution of this part to generalized degree distance is

$$(\sum_{i=1}^{d}(c_i+1)\sum_{i=1}^{d}(c_i-1)-\sum_{i=1}^{d}(c_i^2-1))\cdot 3^\lambda.$$

- We get $d(w_i,w_j)=4$ if and only if w_i and w_j are not the neighbors of the same vertex v_k $(1\leq k\leq d)$. The total contribution of this part to generalized degree distance is

$$2(\binom{n-d}{2}-\sum_{i=1}^{d}\binom{c_i-1}{2})\cdot 4^\lambda.$$

By summing up the above results, we get the desired result. □

In view of Theorem 1, we deduce the following corollaries.

Corollary 1. *The Shultz polynomial of starlike tree $S(c_1, c_2, \cdots, c_d)$ is*

$$
\begin{aligned}
& Sc(S(c_1,c_2,\cdots,c_d),x) \\
= & (\sum_{i=1}^{d}(c_i^2+c_i)+d^2-d)x+(\sum_{i=1}^{d}(2\binom{c_i-1}{2}+(d-1)c_i)+(d+1)(n-d))x^2 \\
& +(\sum_{i=1}^{d}(c_i+1)\sum_{i=1}^{d}(c_i-1)-\sum_{i=1}^{d}(c_i^2-1))x^3+2(\binom{n-d}{2}-\sum_{i=1}^{d}\binom{c_i-1}{2})x^4.
\end{aligned}
$$

Corollary 2. *The additively weighted Harary index (reciprocal degree distance) of starlike tree $S(c_1, c_2, \cdots, c_d)$ is*

$$
\begin{aligned}
& H_A(S(c_1,c_2,\cdots,c_d)) \\
= & (\sum_{i=1}^{d}(c_i^2+c_i)+d^2-d)+\frac{\sum_{i=1}^{d}((\binom{c_i-1}{2}+(d-1)c_i)+(d+1)(n-d)+\binom{n-d}{2})}{2} \\
& +\frac{\sum_{i=1}^{d}(c_i+1)\sum_{i=1}^{d}(c_i-1)-\sum_{i=1}^{d}(c_i^2-1)}{3}.
\end{aligned}
$$

Corollary 3. *The generalized degree distance polynomial of starlike tree $S(c_1, c_2, \cdots, c_d)$ is*

$$
\begin{aligned}
& H_\lambda(S(c_1,c_2,\cdots,c_d),x) \\
= & (\sum_{i=1}^{d}(c_i^2+c_i)+d^2-d)x+(\sum_{i=1}^{d}(2\binom{c_i-1}{2}+(d-1)c_i)+(d+1)(n-d))x^{2^\lambda} \\
& +(\sum_{i=1}^{d}(c_i+1)\sum_{i=1}^{d}(c_i-1)-\sum_{i=1}^{d}(c_i^2-1))x^{3^\lambda}+2(\binom{n-d}{2}-\sum_{i=1}^{d}\binom{c_i-1}{2})x^{4^\lambda}.
\end{aligned}
$$

2.2 Eccentricity related indices of hetrofunctional dendrimer

As macromolecules, hetrofunctional dendrimers $D[n]$ (here n is denoted as the total stage number) have been widely used in pharmacy and medicine. As an example, the structure of $D[6]$ is presented in Figure 2, and the different growth stages are depicted in Figure 3 and Figure 4. Obviously, we have $|V(D[n])| = |E(D[n])| = \begin{cases} 40\times 2^t-38, & \text{if } n=2t \\ 24\times 2^{t+1}-38, & \text{if } n=2t+1, \end{cases}$ where t is a positive integer.

Our proof follows the technology in Farooq et al. [41], and the whole results can be divided into two parts according to the parity of n.

Theorem 2. *If $n = 1$, then*

$$GA_4(D[1]) = 2+\frac{16\sqrt{5}}{9}+\frac{4\sqrt{30}}{11}+\frac{4\sqrt{42}}{13},$$

$$ABC_5(D[1]) = \sqrt{\frac{3}{2}}+2\sqrt{\frac{7}{5}}+2\sqrt{\frac{3}{10}}+2\sqrt{\frac{11}{42}},$$

$$\Pi_1^*(D[1]) = 8^2 9^4 11^2 13^2,$$

$$\Pi_2^*(D[1]) = 16^2 20^4 30^2 42^2,$$

$$Zg_4(D[1]) = 2x^8+4x^9+2x^{11}+2x^{13},$$

$$Zg_6(D[1]) = 2x^{16}+4x^{20}+2x^{30}+2x^{42}.$$

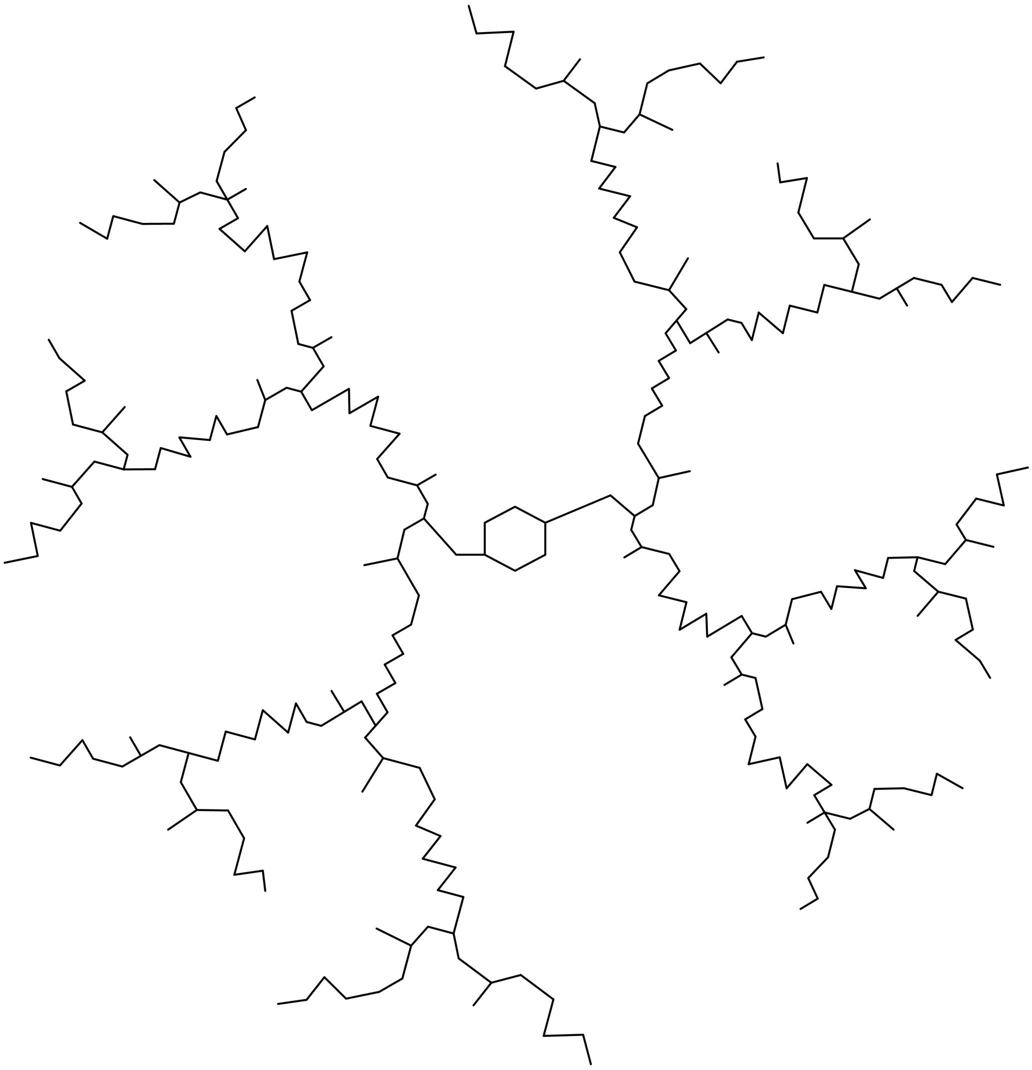

Fig. 2 The structure of $D[6]$

If $n=2$, then

$$\begin{aligned} GA_4(D[2]) &= 2+\frac{16\sqrt{33}}{23}+\frac{8\sqrt{39}}{25}+\frac{4\sqrt{182}}{27}+\frac{8\sqrt{210}}{29}+\frac{32\sqrt{15}}{31} \\ &+\frac{64\sqrt{17}}{33}+\frac{24\sqrt{34}}{35}+\frac{24\sqrt{38}}{37}+\frac{16\sqrt{95}}{39}+\frac{16\sqrt{105}}{41}, \end{aligned}$$

$$\begin{aligned} ABC_5(D[2]) &= 4\sqrt{\frac{5}{121}}+4\sqrt{\frac{7}{44}}+2\sqrt{\frac{23}{156}}+2\sqrt{\frac{25}{182}}+4\sqrt{\frac{9}{70}}+\sqrt{\frac{29}{15}} \\ &+2\sqrt{\frac{31}{17}}+\frac{4}{3}\sqrt{\frac{33}{34}}+\frac{4}{3}\sqrt{\frac{35}{38}}+2\sqrt{\frac{37}{95}}+2\sqrt{\frac{39}{105}}, \end{aligned}$$

$$\Pi_1^*(D[2]) = 22^2 23^4 25^2 27^2 29^4 31^4 33^8 35^4 37^4 39^4 41^4,$$

$$\Pi_2^*(D[2]) = 121^2 132^4 156^2 182^2 210^4 240^4 272^8 306^4 342^4 380^4 420^4,$$

$$Zg_4(D[2]) = 2x^{22}+4x^{23}+2x^{25}+2x^{27}+4x^{29}+4x^{31}+8x^{33}+4x^{35}+4x^{37}+4x^{39}+4x^{41},$$

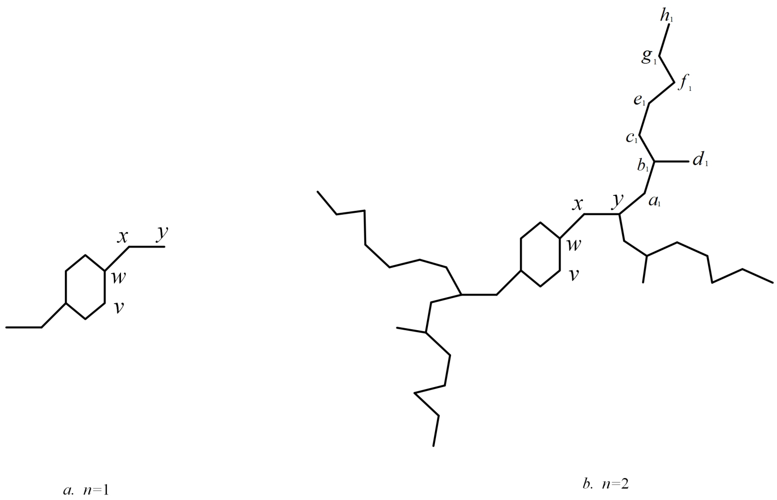

Fig. 3 The core of $D[1]$ and $D[2]$

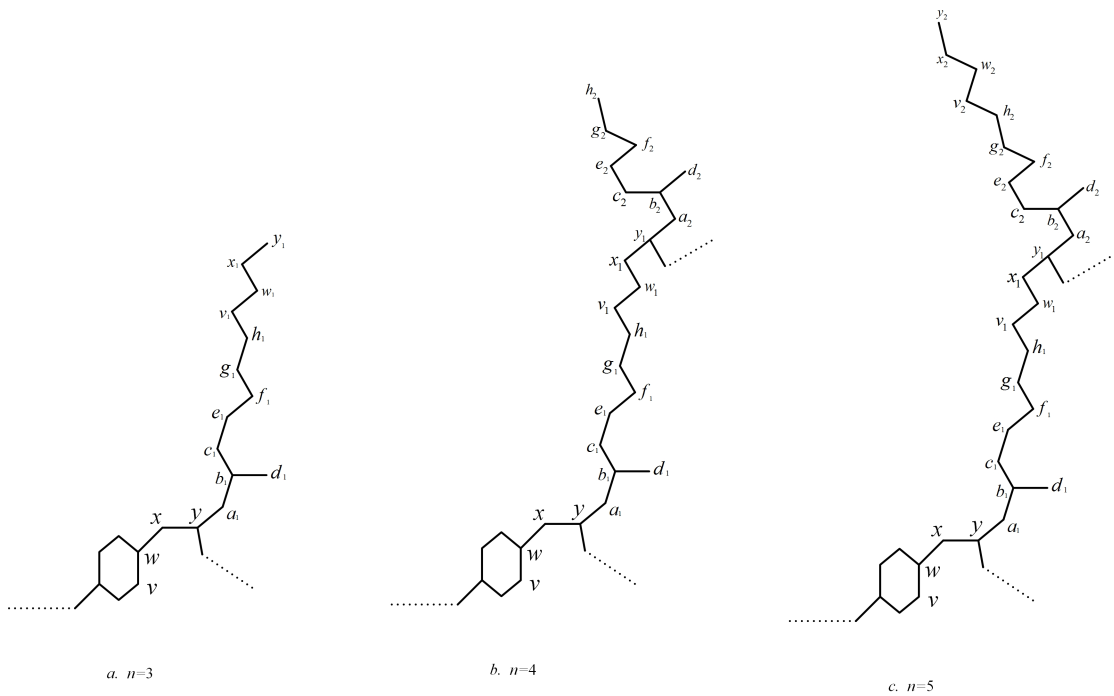

Fig. 4 One branch of $D[3]$, $D[4]$ and $D[5]$

$$Zg_6(D[2]) = 2x^{121} + 4x^{132} + 2x^{156} + 2x^{182} + 4x^{210} + 4x^{240} + 8x^{272} + 4x^{306} + 4x^{342} + 4x^{380} + 4x^{420}.$$

If $n = 3$, then

$$\begin{aligned} GA_4(D[3]) = {} & 2 + \frac{32\sqrt{15}}{31} + \frac{16\sqrt{17}}{33} + \frac{12\sqrt{34}}{35} + \frac{24\sqrt{38}}{37} + \frac{16\sqrt{95}}{39} + \frac{16\sqrt{105}}{41} + \frac{8\sqrt{462}}{43} \\ & + \frac{8\sqrt{506}}{45} + \frac{16\sqrt{138}}{47} + \frac{80\sqrt{6}}{49} + \frac{40\sqrt{26}}{51} + \frac{24\sqrt{78}}{53} + \frac{48\sqrt{21}}{55} + \frac{16\sqrt{203}}{57}, \end{aligned}$$

$$\begin{aligned}ABC_5(D[3]) &= \frac{4}{15}\sqrt{7}+\sqrt{\frac{29}{15}}+\frac{1}{2}\sqrt{\frac{31}{17}}+2\sqrt{\frac{11}{102}}+\frac{4}{3}\sqrt{\frac{35}{38}}+2\sqrt{\frac{37}{95}}+2\sqrt{\frac{13}{35}}+4\sqrt{\frac{41}{462}}\\&+4\sqrt{\frac{43}{506}}+2\sqrt{\frac{13}{46}}+\frac{2}{5}\sqrt{\frac{47}{6}}+\frac{4}{5}\sqrt{\frac{49}{26}}+\frac{4}{3}\sqrt{\frac{17}{26}}+\frac{2}{3}\sqrt{\frac{53}{21}}+2\sqrt{\frac{55}{203}},\end{aligned}$$

$$\Pi_1^*(D[3]) = 30^2 31^4 33^2 35^2 37^4 39^4 41^4 43^4 45^4 47^4 49^4 51^4 53^4 55^4 57^4,$$

$$\Pi_2^*(D[3]) = 225^2 240^4 272^2 306^2 342^4 380^4 420^4 462^4 506^4 552^4 600^4 650^4 702^4 756^4 812^4,$$

$$Zg_4(D[3]) = 2x^{30}+4x^{31}+2x^{33}+2x^{35}+4x^{37}+4x^{39}+4x^{41}+4x^{43}+4x^{45}+4x^{47}+4x^{49}+4x^{51}+4x^{53}+4x^{55}+4x^{57},$$

$$\begin{aligned}Zg_6(D[3]) &= 2x^{225}+4x^{240}+2x^{272}+2x^{306}+4x^{342}+4x^{380}+4x^{420}+4x^{462}+4x^{506}+4x^{552}\\&+4x^{600}+4x^{650}+4x^{702}+4x^{756}+4x^{812}.\end{aligned}$$

If $n \geq 4$ and $n \equiv 0(\mathrm{mod}2)$, then

$$\begin{aligned}GA_4(D[n]) &= 2+\frac{8\sqrt{(11t)\cdot(11t+1)}}{22t+1}+\frac{4\sqrt{(11t+1)\cdot(11t+2)}}{22t+3}\\&+\frac{4\sqrt{(11t+2)\cdot(11t+3)}}{22t+5}+\frac{8\sqrt{(11t+3)\cdot(11t+4)}}{22t+7}\\&+\sum_{i=1}^{t-1}(2^{i+2}\frac{\sqrt{(11t+11i-7)\cdot(11t+11i-6)}}{22t+22i-13}+2^{i+3}\frac{\sqrt{(11t+11i-6)\cdot(11t+11i-5)}}{22t+22i-11}\\&+2^{i+2}\frac{\sqrt{(11t+11i-5)\cdot(11t+11i-4)}}{22t+22i-9}+2^{i+2}\frac{\sqrt{(11t+11i-4)\cdot(11t+11i-3)}}{22t+22i-7}\\&+2^{i+2}\frac{\sqrt{(11t+11i-3)\cdot(11t+11i-2)}}{22t+22i-5}+2^{i+2}\frac{\sqrt{(11t+11i-2)\cdot(11t+11i-1)}}{22t+22i-3}\\&+2^{i+2}\frac{\sqrt{(11t+11i-1)\cdot(11t+11i)}}{22t+22i-1}+2^{i+2}\frac{\sqrt{(11t+11i)\cdot(11t+11i+1)}}{22t+22i+1}\\&+2^{i+2}\frac{\sqrt{(11t+11i+1)\cdot(11t+11i+2)}}{22t+22i+3}+2^{i+2}\frac{\sqrt{(11t+11i+2)\cdot(11t+11i+3)}}{22t+22i+5}\\&+2^{i+2}\frac{\sqrt{(11t+11i+3)\cdot(11t+11i+4)}}{22t+22i+7})+2^{t+2}\frac{\sqrt{(22t-7)\cdot(22t-6)}}{44t-13}\\&+2^{t+3}\frac{\sqrt{(22t-6)\cdot(22t-5)}}{44t-11}+2^{t+2}\frac{\sqrt{(22t-5)\cdot(22t-4)}}{44t-9}+2^{t+2}\frac{\sqrt{(22t-4)\cdot(22t-3)}}{44t-7}\\&+2^{t+2}\frac{\sqrt{(22t-3)\cdot(22t-2)}}{44t-5}+2^{t+2}\frac{\sqrt{(22t-2)\cdot(22t-1)}}{44t-3},\end{aligned}$$

$$ABC_5(D[n]) = \frac{2}{11t}\sqrt{22t-2} + 4\sqrt{\frac{22t-1}{(11t)\cdot(11t+1)}} + 2\sqrt{\frac{22t+1}{(11t+1)\cdot(11t+2)}}$$
$$+2\sqrt{\frac{22t+3}{(11t+2)\cdot(11t+3)}} + 4\sqrt{\frac{22t+5}{(11t+3)\cdot(11t+4)}}$$
$$+\sum_{i=1}^{t-1}(2^{i+1}\sqrt{\frac{22t+22i-15}{(11t+11i-7)\cdot(11t+11i-6)}} + 2^{i+2}\sqrt{\frac{22t+22i-13}{(11t+11i-6)\cdot(11t+11i-5)}}$$
$$+2^{i+1}\sqrt{\frac{22t+22i-11}{(11t+11i-5)\cdot(11t+11i-4)}} + 2^{i+1}\sqrt{\frac{22t+22i-9}{(11t+11i-4)\cdot(11t+11i-3)}}$$
$$+2^{i+1}\sqrt{\frac{22t+22i-7}{(11t+11i-3)\cdot(11t+11i-2)}} + 2^{i+1}\sqrt{\frac{22t+22i-5}{(11t+11i-2)\cdot(11t+11i-1)}}$$
$$+2^{i+1}\sqrt{\frac{22t+22i-3}{(11t+11i-1)\cdot(11t+11i)}} + 2^{i+1}\sqrt{\frac{22t+22i-1}{(11t+11i)\cdot(11t+11i+1)}}$$
$$+2^{i+1}\sqrt{\frac{22t+22i+1}{(11t+11i+1)\cdot(11t+11i+2)}} + 2^{i+1}\sqrt{\frac{22t+22i+3}{(11t+11i+2)\cdot(11t+11i+3)}}$$
$$+2^{i+1}\sqrt{\frac{22t+22i+5}{(11t+11i+3)\cdot(11t+11i+4)}}) + 2^{t+1}\sqrt{\frac{44t-15}{(22t-7)\cdot(22t-6)}}$$
$$+2^{t+2}\sqrt{\frac{44t-13}{(22t-6)\cdot(22t-5)}}) + 2^{t+1}\sqrt{\frac{44t-11}{(22t-5)\cdot(22t-4)}}$$
$$+2^{t+1}\sqrt{\frac{44t-9}{(22t-4)\cdot(22t-3)}} + 2^{t+1}\sqrt{\frac{44t-7}{(22t-3)\cdot(22t-2)}}$$
$$+2^{t+1}\sqrt{\frac{44t-5}{(22t-2)\cdot(22t-1)}},$$

$$\Pi_1^*(D[n]) = (22t)^2(22t+1)^4(22t+3)^2(22t+5)^2(22t+7)^4\cdot\prod_{i=1}^{t-1}((22t+22i-13)^{2^{i+1}}$$
$$(22t+22i-11)^{2^{i+2}}(22t+22i-9)^{2^{i+1}}(22t+22i-7)^{2^{i+1}}(22t+22i-5)^{2^{i+1}}$$
$$\cdot(22t+22i-3)^{2^{i+1}}(22t+22i-1)^{2^{i+1}}(22t+22i+1)^{2^{i+1}}(22t+22i+3)^{2^{i+1}}$$
$$\cdot(22t+22i+5)^{2^{i+1}}(22t+22i+7)^{2^{i+1}})(44t-13)^{2^{t+1}}(44t-11)^{2^{t+2}}(44t-9)^{2^{t+1}}$$
$$\cdot(44t-7)^{2^{t+1}}(44t-5)^{2^{t+1}}(44t-3)^{2^{t+1}},$$

$$\Pi_2^*(D[n]) = (11t)^8(11t+1)^6(11t+2)^4(11t+3)^6(11t+4)^4\cdot\prod_{i=1}^{t-1}((11t+11i-7)^{2^{i+1}}$$
$$\cdot(11t+11i-6))^{3\cdot 2^{i+1}}(11t+11i-5)^{3\cdot 2^{i+1}}(11t+11i-4)^{2^{i+2}}(11t+11i-3)^{2^{i+2}}(11t+11i-2)^{2^{i+2}}$$
$$\cdot(11t+11i-1)^{2^{i+2}}(11t+11i)^{2^{i+2}}(11t+11i+1)^{2^{i+2}}(11t+11i+2)^{2^{i+2}}(11t+11i+3)^{2^{i+2}}$$
$$\cdot(11t+11i+4)^{2^{i+1}})(22t-7)^{2^{t+1}}(22t-6)^{3\cdot 2^{t+1}}(22t-5)^{3\cdot 2^{t+1}}(22t-4)^{2^{t+2}}(22t-3)^{2^{t+2}}$$
$$\cdot(22t-2)^{2^{t+2}}(22t-1)^{2^{t+1}},$$

$$Zg_4(D[n]) = 2x^{22t} + 4x^{22t+1} + 2x^{22t+3} + 2x^{22t+5} + 4x^{22t+7} + \sum_{i=1}^{t-1}(2^{i+1}x^{22t+22i-13}$$
$$+2^{i+2}x^{22t+22i-11} + 2^{i+1}x^{22t+22i-9} + 2^{i+1}x^{22t+22i-7} + 2^{i+1}x^{22t+22i-5}$$
$$+2^{i+1}x^{22t+22i-3} + 2^{i+1}x^{22t+22i-1} + 2^{i+1}x^{22t+22i+1} + 2^{i+1}x^{22t+22i+3} + 2^{i+1}x^{22t+22i+5}$$
$$+2^{i+1}x^{22t+22i+7}) + 2^{t+1}x^{44t-13} + 2^{t+2}x^{44t-11} + 2^{t+1}x^{44t-9}$$
$$+2^{t+1}x^{44t-7} + 2^{t+1}x^{44t-5} + 2^{t+1}x^{44t-3},$$

$$Zg_6(D[n]) = 2x^{(11t)\cdot(11t)} + 4x^{(11t)\cdot(11t+1)} + 2x^{(11t+1)\cdot(11t+2)} + 2x^{(11t+2)\cdot(11t+3)}$$
$$+4x^{(11t+3)\cdot(11t+4)} + \sum_{i=1}^{t-1}(2^{i+1}x^{(11t+11i-7)\cdot(11t+11i-6)} + 2^{i+2}x^{(11t+11i-6)(11t+11i-5)}$$
$$+2^{i+1}x^{(11t+11i-5)\cdot(11t+11i-4)} + 2^{i+1}x^{(11t+11i-4)\cdot(11t+11i-3)} + 2^{i+1}x^{(11t+11i-3)\cdot(11t+11i-2)}$$
$$+2^{i+1}x^{(11t+11i-2)\cdot(11t+11i-1)} + 2^{i+1}x^{(11t+11i-1)\cdot(11t+11i)} + 2^{i+1}x^{(11t+11i)\cdot(11t+11i+1)}$$
$$+2^{i+1}x^{(11t+11i+1)\cdot(11t+11i+2)} + 2^{i+1}x^{(11t+11i+2)\cdot(11t+11i+3)} + 2^{i+1}x^{(11t+11i+3)\cdot(11t+11i+4)})$$
$$+2^{t+1}x^{(22t-7)\cdot(22t-6)} + 2^{t+2}x^{(22t-6)\cdot(22t-5)} + 2^{t+1}x^{(22t-5)\cdot(22t-4)}$$
$$+2^{t+1}x^{(22t-4)\cdot(22t-3)} + 2^{t+1}x^{(22t-3)\cdot(22t-2)} + 2^{t+1}x^{(22t-2)\cdot(22t-1)}.$$

If $n \geq 5$ and $n \equiv 1(\mathrm{mod}2)$, then

$$GA_4(D[n]) = 2 + \frac{8\sqrt{(11t+4)\cdot(11t+5)}}{22t+9}$$
$$+\frac{4\sqrt{(11t+5)\cdot(11t+6)}}{22t+11} + \frac{4\sqrt{(11t+6)\cdot(11t+7)}}{22t+13} + \frac{8\sqrt{(11t+7)\cdot(11t+8)}}{22t+15}$$
$$+\frac{8\sqrt{(11t+8)\cdot(11t+9)}}{22t+17} + \frac{16\sqrt{(11t+9)\cdot(11t+10)}}{22t+19} + \frac{8\sqrt{(11t+10)\cdot(11t+11)}}{22t+21}$$
$$+\frac{8\sqrt{(11t+11)\cdot(11t+12)}}{22t+23} + \frac{8\sqrt{(11t+12)\cdot(11t+13)}}{22t+25} + \frac{8\sqrt{(11t+13)\cdot(11t+14)}}{22t+27}$$
$$+\frac{8\sqrt{(11t+14)\cdot(11t+15)}}{22t+29} + \frac{8\sqrt{(11t+15)\cdot(11t+16)}}{22t+31} + \frac{8\sqrt{(11t+16)\cdot(11t+17)}}{22t+33}$$
$$+\frac{8\sqrt{(11t+17)\cdot(11t+18)}}{22t+35} + \sum_{i=1}^{t-1}(2^{i+3}\frac{\sqrt{(11t+11i+7)\cdot(11t+11i+8)}}{22t+22i+15}$$
$$+2^{i+3}\frac{\sqrt{(11t+11i+8)\cdot(11t+11i+9)}}{22t+22i+17} + 2^{i+4}\frac{\sqrt{(11t+11i+9)\cdot(11t+11i+10)}}{22t+22i+19}$$
$$+2^{i+3}\frac{\sqrt{(11t+11i+10)\cdot(11t+11i+11)}}{22t+22i+21} + 2^{i+3}\frac{\sqrt{(11t+11i+11)\cdot(11t+11i+12)}}{22t+22i+23}$$
$$+2^{i+3}\frac{\sqrt{(11t+11i+12)\cdot(11t+11i+13)}}{22t+22i+25} + 2^{i+3}\frac{\sqrt{(11t+11i+13)\cdot(11t+11i+14)}}{22t+22i+27}$$
$$+2^{i+3}\frac{\sqrt{(11t+11i+14)\cdot(11t+11i+15)}}{22t+22i+29} + 2^{i+3}\frac{\sqrt{(11t+11i+15)\cdot(11t+11i+16)}}{22t+22i+31}$$
$$+2^{i+3}\frac{\sqrt{(11t+11i+16)\cdot(11t+11i+17)}}{22t+22i+33} + 2^{i+3}\frac{\sqrt{(11t+11i+17)\cdot(11t+11i+18)}}{22t+22i+35}),$$

$$\begin{aligned}
ABC_5(D[n]) &= \frac{2}{11t+4}\sqrt{22t+6}+4\sqrt{\frac{22t+7}{(11t+4)\cdot(11t+5)}}\\
&+2\sqrt{\frac{22t+9}{(11t+5)\cdot(11t+6)}}+2\sqrt{\frac{22t+11}{(11t+6)\cdot(11t+7)}}+4\sqrt{\frac{22t+13}{(11t+7)\cdot(11t+8)}}\\
&+4\sqrt{\frac{22t+15}{(11t+8)\cdot(11t+9)}}+8\sqrt{\frac{22t+17}{(11t+9)\cdot(11t+10)}}+4\sqrt{\frac{22t+19}{(11t+10)\cdot(11t+11)}}\\
&+4\sqrt{\frac{22t+21}{(11t+11)\cdot(11t+12)}}+4\sqrt{\frac{22t+23}{(11t+12)\cdot(11t+13)}}+4\sqrt{\frac{22t+25}{(11t+13)\cdot(11t+14)}}\\
&+4\sqrt{\frac{22t+27}{(11t+14)\cdot(11t+15)}}+4\sqrt{\frac{22t+29}{(11t+15)\cdot(11t+16)}}+4\sqrt{\frac{22t+31}{(11t+16)\cdot(11t+17)}}\\
&+4\sqrt{\frac{22t+33}{(11t+17)\cdot(11t+18)}}+\sum_{i=1}^{t-1}(2^{i+2}\sqrt{\frac{22t+22i+13}{(11t+11i+7)\cdot(11t+11i+8)}}\\
&+2^{i+2}\sqrt{\frac{22t+22i+15}{(11t+11i+8)\cdot(11t+11i+9)}}+2^{i+3}\sqrt{\frac{22t+22i+17}{(11t+11i+9)\cdot(11t+11i+10)}}\\
&+2^{i+2}\sqrt{\frac{22t+22i+19}{(11t+11i+10)\cdot(11t+11i+11)}}+2^{i+2}\sqrt{\frac{22t+22i+21}{(11t+11i+11)\cdot(11t+11i+12)}}\\
&+2^{i+2}\sqrt{\frac{22t+22i+23}{(11t+11i+12)\cdot(11t+11i+13)}}+2^{i+2}\sqrt{\frac{22t+22i+25}{(11t+11i+13)\cdot(11t+11i+14)}}\\
&+2^{i+2}\sqrt{\frac{22t+22i+27}{(11t+11i+14)\cdot(11t+11i+15)}}+2^{i+2}\sqrt{\frac{22t+22i+29}{(11t+11i+15)\cdot(11t+11i+16)}}\\
&+2^{i+2}\sqrt{\frac{22t+22i+31}{(11t+11i+16)\cdot(11t+11i+17)}}+2^{i+2}\sqrt{\frac{22t+22i+33}{(11t+11i+17)\cdot(11t+11i+18)}}),
\end{aligned}$$

$$\begin{aligned}
&\Pi_1^*(D[n]) = (22t+8)^2(22t+9)^4(22t+11)^2(22t+13)^2(22t+15)^4(22t+17)^4\\
&\cdot(22t+19)^8(22t+21)^4(22t+23)^4(22t+25)^4(22t+27)^4(22t+29)^4(22t+31)^4(22t+33)^4(22t+35)^4\\
&\cdot\prod_{i=1}^{t-1}((22t+22i+15)^{2^{i+2}}(22t+22i+17)^{2^{i+2}}(22t+22i+19)^{2^{i+3}}\\
&\cdot(22t+22i+21)^{2^{i+2}}(22t+22i+23)^{2^{i+2}}(22t+22i+25)^{2^{i+2}}(22t+22i+27)^{2^{i+2}}\\
&\cdot(22t+22i+29)^{2^{i+2}}(22t+22i+31)^{2^{i+2}}(22t+22i+33)^{2^{i+2}}(22t+22i+35)^{2^{i+2}}),
\end{aligned}$$

$$\begin{aligned}
&\Pi_2^*(D[n]) = (11t+4)^8(11t+5)^6(11t+6)^4(11t+7)^6(11t+8)^8(11t+9)^{12}(11t+10)^{12}\\
&\cdot(11t+11)^8(11t+12)^8(11t+13)^8(11t+14)^8(11t+15)^8(11t+16)^8(11t+17)^8(11t+18)^4\\
&\cdot\prod_{i=1}^{t-1}((11t+11i+7)^{2^{i+2}}(11t+11i+8))^{2^{i+3}}(11t+11i+9))^{3\cdot 2^{i+2}}(11t+11i+10)^{3\cdot 2^{i+2}}\\
&\cdot(11t+11i+11)^{2^{i+3}}(11t+11i+12)^{2^{i+3}}(11t+11i+13)^{2^{i+3}}(11t+11i+14)^{2^{i+3}}\\
&\cdot(11t+11i+15)^{2^{i+3}}(11t+11i+16)^{2^{i+3}}(11t+11i+17)^{2^{i+3}}(11t+11i+18)^{2^{i+2}}),
\end{aligned}$$

$$Zg_4(D[n]) = 2x^{22t+8} + 4x^{22t+9} + 2x^{22t+11} + 2x^{22t+13} + 4x^{22t+15}$$
$$+4x^{22t+17} + 8x^{22t+19} + 4x^{22t+21} + 4x^{22t+23} + 4x^{22t+25} + 4x^{22t+27}$$
$$+4x^{22t+29} + 4x^{22t+31} + 4x^{22t+33} + 4x^{22t+35} + \sum_{i=1}^{t-1}(2^{i+2}x^{22t+22i+15}$$
$$+2^{i+2}x^{22t+22i+17} + 2^{i+3}x^{22t+22i+19} + 2^{i+2}x^{22t+22i+21} + 2^{i+2}x^{22t+22i+23}$$
$$+2^{i+2}x^{22t+22i+25} + 2^{i+2}x^{22t+22i+27} + 2^{i+2}x^{22t+22i+29} + 2^{i+2}x^{22t+22i+31}$$
$$+2^{i+2}x^{22t+22i+33} + 2^{i+2}x^{22t+22i+35}),$$

$$Zg_6(D[n]) = 2x^{(11t+4)\cdot(11t+4)} + 4x^{(11t+4)\cdot(11t+5)} + 2x^{(11t+5)\cdot(11t+6)}$$
$$+2x^{(11t+6)\cdot(11t+7)} + 4x^{(11t+7)\cdot(11t+8)} + 4x^{(11t+8)\cdot(11t+9)} + 8x^{(11t+9)\cdot(11t+10)}$$
$$+4x^{(11t+10)\cdot(11t+11)} + 4x^{(11t+11)\cdot(11t+12)} + 4x^{(11t+12)\cdot(11t+13)} + 4x^{(11t+13)\cdot(11t+14)}$$
$$+4x^{(11t+14)\cdot(11t+15)} + 4x^{(11t+15)\cdot(11t+16)} + 4x^{(11t+16)\cdot(11t+17)} + 4x^{(11t+17)\cdot(11t+18)}$$
$$+\sum_{i=1}^{t-1}(2^{i+2}x^{(11t+11i+7)\cdot(11t+11i+8)} + 2^{i+2}x^{(11t+11i+8)\cdot(11t+11i+9)} + 2^{i+3}x^{(11t+11i+9)\cdot(11t+11i+10)}$$
$$+2^{i+2}x^{(11t+11i+10)\cdot(11t+11i+11)} + 2^{i+2}x^{(11t+11i+11)\cdot(11t+11i+12)} + 2^{i+2}x^{(11t+11i+12)\cdot(11t+11i+13)}$$
$$+2^{i+2}x^{(11t+11i+13)\cdot(11t+11i+14)} + 2^{i+2}x^{(11t+11i+14)\cdot(11t+11i+15)} + 2^{i+2}x^{(11t+11i+15)\cdot(11t+11i+16)}$$
$$+2^{i+2}x^{(11t+11i+16)\cdot(11t+11i+17)} + 2^{i+2}x^{(11t+11i+17)\cdot(11t+11i+18)}).$$

Proof. Since $D[n]$ is symmetrical, we can mark the vertices several representative symbols which are described in Figure 3 and Figure 4. Next, we only present the detailed proof of GA_4 index, and other parts of result can be yielded in the similar way.

If $n \equiv 1(\text{mod}2)$, then let $t = \frac{n-1}{2}$ and $1 \le i \le t-1$. By the analysis of graph structure of $D[n]$, the set of $E(D[n])$ can be divided into the following subsets which are described as follows:

- (u,v): with eccentricities $11t+4$ and $11t+4$, and there are two edges in this class;
- (v,w): with eccentricities $11t+4$ and $11t+5$, and there are four edges in this class;
- (w,x): with eccentricities $11t+5$ and $11t+6$, and there are two edges in this class;
- (x,y): with eccentricities $11t+6$ and $11t+7$, and there are two edges in this class;
- (y,a_1): with eccentricities $11t+7$ and $11t+8$, and there are four edges in this class;
- (a_1,b_1): with eccentricities $11t+8$ and $11t+9$, and there are four edges in this class;
- (b_1,c_1): with eccentricities $11t+9$ and $11t+10$, and there are eight edges in this class;
- (c_1,e_1): with eccentricities $11t+10$ and $11t+11$, and there are four edges in this class;
- (e_1,f_1): with eccentricities $11t+11$ and $11t+12$, and there are four edges in this class;
- (f_1,g_1): with eccentricities $11t+12$ and $11t+13$, and there are four edges in this class;
- (g_1,h_1): with eccentricities $11t+13$ and $11t+14$, and there are four edges in this class;
- (h_1,v_1): with eccentricities $11t+14$ and $11t+15$, and there are four edges in this class;
- (v_1,w_1): with eccentricities $11t+15$ and $11t+16$, and there are four edges in this class;

- (w_1, x_1): with eccentricities $11t+16$ and $11t+17$, and there are four edges in this class;
- (x_1, y_1): with eccentricities $11t+17$ and $11t+18$, and there are four edges in this class;
- (y_i, a_{i+1}): with eccentricities $11t+11i+7$ and $11t+11i+8$, and there are 2^{i+2} edges in this class;
- (a_{i+1}, b_{i+1}): with eccentricities $11t+11i+8$ and $11t+11i+9$, and there are 2^{i+2} edges in this class;
- (b_{i+1}, c_{i+1}): with eccentricities $11t+11i+9$ and $11t+11i+10$, and there are 2^{i+3} edges in this class;
- (c_{i+1}, e_{i+1}): with eccentricities $11t+11i+10$ and $11t+11i+11$, and there are 2^{i+2} edges in this class;
- (e_{i+1}, f_{i+1}): with eccentricities $11t+11i+11$ and $11t+11i+12$, and there are 2^{i+2} edges in this class;
- (f_{i+1}, g_{i+1}): with eccentricities $11t+11i+12$ and $11t+11i+13$, and there are 2^{i+2} edges in this class;
- (g_{i+1}, h_{i+1}): with eccentricities $11t+11i+13$ and $11t+11i+14$, and there are 2^{i+2} edges in this class;
- (h_{i+1}, v_{i+1}): with eccentricities $11t+11i+14$ and $11t+11i+15$, and there are 2^{i+2} edges in this class;
- (v_{i+1}, w_{i+1}): with eccentricities $11t+11i+15$ and $11t+11i+16$, and there are 2^{i+2} edges in this class;
- (w_{i+1}, x_{i+1}): with eccentricities $11t+11i+16$ and $11t+11i+17$, and there are 2^{i+2} edges in this class;
- (x_{i+1}, y_{i+1}): with eccentricities $11t+11i+17$ and $11t+11i+18$, and there are 2^{i+2} edges in this class.

If $t=0$, then $n=1$, we have

$$GA_4(D[1]) = \sum_{uv\in E(D[1])} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)} = 2\frac{2\sqrt{4\cdot 4}}{4+4} + 4\frac{2\sqrt{4\cdot 5}}{4+5} + 2\frac{2\sqrt{5\cdot 6}}{5+6} + 2\frac{2\sqrt{6\cdot 7}}{6+7}.$$

If $t=1$, then $n=3$, we get

$$\begin{aligned} GA_4(D[3]) &= \sum_{uv\in E(D[3])} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)} \\ &= 2\frac{2\sqrt{15\cdot 15}}{15+15} + 4\frac{2\sqrt{15\cdot 16}}{15+16} + 2\frac{2\sqrt{16\cdot 17}}{16+17} + 2\frac{2\sqrt{17\cdot 18}}{17+18} + 4\frac{2\sqrt{18\cdot 19}}{18+19} \\ &\quad + 4\frac{2\sqrt{19\cdot 20}}{19+20} + 4\frac{2\sqrt{20\cdot 21}}{20+21} + 4\frac{2\sqrt{21\cdot 22}}{21+22} + 4\frac{2\sqrt{22\cdot 23}}{22+23} + 4\frac{2\sqrt{23\cdot 24}}{23+24} \\ &\quad + 4\frac{2\sqrt{24\cdot 25}}{24+25} + 4\frac{2\sqrt{25\cdot 26}}{25+26} + 4\frac{2\sqrt{26\cdot 27}}{26+27} + 4\frac{2\sqrt{27\cdot 28}}{27+28} + 4\frac{2\sqrt{28\cdot 29}}{28+29}. \end{aligned}$$

If $n \geq 5$, then we obtain

$$
\begin{aligned}
GA_4(D[n]) = &\sum_{uv\in E(D[n])} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)} = 2\frac{2\sqrt{(11t+4)\cdot(11t+4)}}{(11t+4)+(11t+4)} + 4\frac{2\sqrt{(11t+4)\cdot(11t+5)}}{(11t+4)+(11t+5)} \\
&+2\frac{2\sqrt{(11t+5)\cdot(11t+6)}}{(11t+5)+(11t+6)} + 2\frac{2\sqrt{(11t+6)\cdot(11t+7)}}{(11t+6)+(11t+7)} + 4\frac{2\sqrt{(11t+7)\cdot(11t+8)}}{(11t+7)+(11t+8)} \\
&+4\frac{2\sqrt{(11t+8)\cdot(11t+9)}}{(11t+8)+(11t+9)} + 8\frac{2\sqrt{(11t+9)\cdot(11t+10)}}{(11t+9)+(11t+10)} + 4\frac{2\sqrt{(11t+10)\cdot(11t+11)}}{(11t+10)+(11t+11)} \\
&+4\frac{2\sqrt{(11t+11)\cdot(11t+12)}}{(11t+11)+(11t+12)} + 4\frac{2\sqrt{(11t+12)\cdot(11t+13)}}{(11t+12)+(11t+13)} + 4\frac{2\sqrt{(11t+13)\cdot(11t+14)}}{(11t+13)+(11t+14)} \\
&+4\frac{2\sqrt{(11t+14)\cdot(11t+15)}}{(11t+14)+(11t+15)} + 4\frac{2\sqrt{(11t+15)\cdot(11t+16)}}{(11t+15)+(11t+16)} + 4\frac{2\sqrt{(11t+16)\cdot(11t+17)}}{(11t+16)+(11t+17)} \\
&+4\frac{2\sqrt{(11t+17)\cdot(11t+18)}}{(11t+17)+(11t+18)} + \sum_{i=1}^{t-1}(2^{i+2}\frac{2\sqrt{(11t+11i+7)\cdot(11t+11i+8)}}{(11t+11i+7)+(11t+11i+8)} \\
&+2^{i+2}\frac{2\sqrt{(11t+11i+8)\cdot(11t+11i+9)}}{(11t+11i+8)+(11t+11i+9)} + 2^{i+3}\frac{2\sqrt{(11t+11i+9)\cdot(11t+11i+10)}}{(11t+11i+9)+(11t+11i+10)} \\
&+2^{i+2}\frac{2\sqrt{(11t+11i+10)\cdot(11t+11i+11)}}{(11t+11i+10)+(11t+11i+11)} + 2^{i+2}\frac{2\sqrt{(11t+11i+11)\cdot(11t+11i+12)}}{(11t+11i+11)+(11t+11i+12)} \\
&+2^{i+2}\frac{2\sqrt{(11t+11i+12)\cdot(11t+11i+13)}}{(11t+11i+12)+(11t+11i+13)} + 2^{i+2}\frac{2\sqrt{(11t+11i+13)\cdot(11t+11i+14)}}{(11t+11i+13)+(11t+11i+14)} \\
&+2^{i+2}\frac{2\sqrt{(11t+11i+14)\cdot(11t+11i+15)}}{(11t+11i+14)+(11t+11i+15)} + 2^{i+2}\frac{2\sqrt{(11t+11i+15)\cdot(11t+11i+16)}}{(11t+11i+15)+(11t+11i+16)} \\
&+2^{i+2}\frac{2\sqrt{(11t+11i+16)\cdot(11t+11i+17)}}{(11t+11i+16)+(11t+11i+17)} + 2^{i+2}\frac{2\sqrt{(11t+11i+17)\cdot(11t+11i+18)}}{(11t+11i+17)+(11t+11i+18)}).
\end{aligned}
$$

If $n \equiv 0(\text{mod}2)$, then let $t = \frac{n}{2}$ and $1 \leq i \leq t-1$. According to the analysis of molecular structure of $D[n]$, the edge set of $D[n]$ can be divided into the following subsets which are presented as follows:

- (u,v): with eccentricities $11t$ and $11t$, and there are two edges in this class;
- (v,w): with eccentricities $11t$ and $11t+1$, and there are four edges in this class;
- (w,x): with eccentricities $11t+1$ and $11t+2$, and there are two edges in this class;
- (x,y): with eccentricities $11t+2$ and $11t+3$, and there are two edges in this class;
- (y,a_1): with eccentricities $11t+3$ and $11t+4$, and there are four edges in this class;
- (a_i,b_i): with eccentricities $11t+11i-7$ and $11t+11i-6$, and there are 2^{i+1} edges in this class;
- (b_i,c_i): with eccentricities $11t+11i-6$ and $11t+11i-5$, and there are 2^{i+2} edges in this class;
- (c_i,e_i): with eccentricities $11t+11i-5$ and $11t+11i-4$, and there are 2^{i+1} edges in this class;
- (e_i,f_i): with eccentricities $11t+11i-4$ and $11t+11i-3$, and there are 2^{i+1} edges in this class;
- (f_i,g_i): with eccentricities $11t+11i-3$ and $11t+11i-2$, and there are 2^{i+1} edges in this class;
- (g_i,h_i): with eccentricities $11t+11i-2$ and $11t+11i-1$, and there are 2^{i+1} edges in this class;

- (h_i, v_i): with eccentricities $11t+11i-1$ and $11t+11i$, and there are 2^{i+1} edges in this class;
- (v_i, w_i): with eccentricities $11t+11i$ and $11t+11i+1$, and there are 2^{i+1} edges in this class;
- (w_i, x_i): with eccentricities $11t+11i+1$ and $11t+11i+2$, and there are 2^{i+1} edges in this class;
- (x_i, y_i): with eccentricities $11t+11i+2$ and $11t+11i+3$, and there are 2^{i+1} edges in this class;
- (y_i, a_{i+1}): with eccentricities $11t+11i+3$ and $11t+11i+4$, and there are 2^{i+2} edges in this class;
- (a_t, b_t): with eccentricities $22t-7$ and $22t-6$, and there are 2^{t+1} edges in this class;
- (b_t, c_t): with eccentricities $22t-6$ and $22t-5$, and there are 2^{t+2} edges in this class;
- (c_t, e_t): with eccentricities $22t-5$ and $22t-4$, and there are 2^{t+1} edges in this class;
- (e_t, f_t): with eccentricities $22t-4$ and $22t-3$, and there are 2^{t+1} edges in this class;
- (f_t, g_t): with eccentricities $22t-3$ and $22t-2$, and there are 2^{t+1} edges in this class;
- (g_t, h_t): with eccentricities $22t-2$ and $22t-1$, and there are 2^{t+1} edges in this class.

If $t=1$, then $n=2$, we have

$$
\begin{aligned}
GA_4(D[2]) = \sum_{uv\in E(D[2])} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)} &= 2\frac{2\sqrt{11\cdot 11}}{11+11} + 4\frac{2\sqrt{11\cdot 12}}{11+12} + 2\frac{2\sqrt{12\cdot 13}}{12+13} + 2\frac{2\sqrt{13\cdot 14}}{13+14} \\
&+ 4\frac{2\sqrt{14\cdot 15}}{14+15} + 4\frac{2\sqrt{15\cdot 16}}{15+16} + 8\frac{2\sqrt{16\cdot 17}}{16+17} + 4\frac{2\sqrt{17\cdot 18}}{17+18} + 4\frac{2\sqrt{18\cdot 19}}{18+19} + 4\frac{2\sqrt{19\cdot 20}}{19+20} + 4\frac{2\sqrt{20\cdot 21}}{20+21}.
\end{aligned}
$$

If $n \geq 4$, then we obtain

$$
\begin{aligned}
GA_4(D[n]) &= \sum_{uv\in E(D[n])} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)} = 2\frac{2\sqrt{(11t)\cdot(11t)}}{(11t)+(11t)} + 4\frac{2\sqrt{(11t)\cdot(11t+1)}}{(11t)+(11t+1)} \\
&+2\frac{2\sqrt{(11t+1)\cdot(11t+2)}}{(11t+1)+(11t+2)} + 2\frac{2\sqrt{(11t+2)\cdot(11t+3)}}{(11t+2)+(11t+3)} + 4\frac{2\sqrt{(11t+3)\cdot(11t+4)}}{(11t+3)+(11t+4)} \\
&+\sum_{i=1}^{t-1}(2^{i+1}\frac{2\sqrt{(11t+11i-7)\cdot(11t+11i-6)}}{(11t+11i-7)+(11t+11i-6)} + 2^{i+2}\frac{2\sqrt{(11t+11i-6)\cdot(11t+11i-5)}}{(11t+11i-6)+(11t+11i-5)} \\
&+2^{i+1}\frac{2\sqrt{(11t+11i-5)\cdot(11t+11i-4)}}{(11t+11i-5)+(11t+11i-4)} + 2^{i+1}\frac{2\sqrt{(11t+11i-4)\cdot(11t+11i-3)}}{(11t+11i-4)+(11t+11i-3)} \\
&+2^{i+1}\frac{2\sqrt{(11t+11i-3)\cdot(11t+11i-2)}}{(11t+11i-3)+(11t+11i-2)} + 2^{i+1}\frac{2\sqrt{(11t+11i-2)\cdot(11t+11i-1)}}{(11t+11i-2)+(11t+11i-1)} \\
&+2^{i+1}\frac{2\sqrt{(11t+11i-1)\cdot(11t+11i)}}{(11t+11i-1)+(11t+11i)} + 2^{i+1}\frac{2\sqrt{(11t+11i)\cdot(11t+11i+1)}}{(11t+11i)+(11t+11i+1)} \\
&+2^{i+1}\frac{2\sqrt{(11t+11i+1)\cdot(11t+11i+2)}}{(11t+11i+1)+(11t+11i+2)} + 2^{i+1}\frac{2\sqrt{(11t+11i+2)\cdot(11t+11i+3)}}{(11t+11i+2)+(11t+11i+3)} \\
&+2^{i+1}\frac{2\sqrt{(11t+11i+3)\cdot(11t+11i+4)}}{(11t+11i+3)+(11t+11i+4)}) + 2^{t+1}\frac{2\sqrt{(22t-7)\cdot(22t-6)}}{(22t-7)+(22t-6)} \\
&+2^{t+2}\frac{2\sqrt{(22t-6)\cdot(22t-5)}}{(22t-6)+(22t-5)} + 2^{t+1}\frac{2\sqrt{(22t-5)\cdot(22t-4)}}{(22t-5)+(22t-4)} \\
&+2^{t+1}\frac{2\sqrt{(22t-4)\cdot(22t-3)}}{(22t-4)+(22t-3)} + 2^{t+1}\frac{2\sqrt{(22t-3)\cdot(22t-2)}}{(22t-3)+(22t-2)} \\
&+2^{t+1}\frac{2\sqrt{(22t-2)\cdot(22t-1)}}{(22t-2)+(22t-1)}.
\end{aligned}
$$

Thus, we yield the expected result. □

3 Conclusion

In this paper, we mainly discuss two molecular graphs which commonly appeared in drug structures. Our results can be concluded as follows: first, we manifest the generalized degree distance of starlike tree; second, we report the eccentricity related indices of hetrofunctional dendrimer. Since these indices are widely used in the analysis of chemical and pharmacological properties of drugs, the theoretical results obtained in our article admit promising prospects of engineering applications in the field of chemistry, pharmacy and medical science.

4 Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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