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Generalized atom-bond connectivity analysis of several chemical molecular graphs

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Lots of drug tests show strong inner relationships between the bio-medical and pharmacological characteristics of the drugs and their molecular structures. Due to the effectiveness for pharmaceutical and medical scientists of their ability to grasp the biological and chemical characteristics of new drugs, the generalized atom-bond connectivity index was defined to analyze the drug molecular structures. The analysis should find widespread application prospects in developing countries, especially in poor places without the adequate financial ability and affordability of much needed chemical reagents and equipment. In this paper, based on the drug molecular structure analysis and driving edge technology, we propose the generalized atom-bond connectivity index of several popular chemical structures which is quite common in drug molecular graphs.

Keywords Computational chemical; Generalized atom-bond connectivity index; dendrimer stars; bridge graph; benzenoid series

INTRODUCTION

A wide range of new drugs emerge each year with the rapid development of the manufacture of medicines. Therefore, lots of work is needed to determine the pharmacological, chemical and biological characteristics of these new drugs. The relevant reagent equipment and lab assistants are in demand in order to test the performance and side effects of these new drugs. However, in some poor areas (such as the countries in South America, Africa and Southeast Asia), they are not rich enough to afford the reagents and equipment necessary to assess the biochemical properties. Luckily, we can refer to the contributions of relevant previous studies, for example, the chemical and pharmacodynamics characteristics of the drugs and their molecular structures as these are closely linked. Once the indicators of these drug molecular structures are calculated in view of defining their topological indices, these can be used to understand their medical properties and help to repair and make up for all the defects of the medicine following the chemical experiments. From this point of view, we can appreciate the effectiveness of the methods on the topological index of computation especially for developing countries, where the available biological and medical information about new drugs may be easily obtained without the need to carry out chemical experiments and purchase expensive hardware.

Traditionally, we look upon the structure of a drug as an undirected graph in the mathematical model of a given medicine. Each vertex represents an atom in the graph and the chemical bond between these atoms is represented by each edge. We consider G as a simple graph corresponding to a drug structure with an atom (vertex) set as $V(G)$ and a chemical bond (edge) set as $E(G)$. A topological index defined on the molecule structure G can be regarded as a real-valued function f: $G \to R^+$ which maps each drug molecular structure to certain real numbers. Decades ago, scientists introduced significant indices, including the Wiener index, the PI index, the Zagreb index and the eccentric index, to measure the characters of the drug molecules. Some reports help to determine these topological indices of special molecular graphs in chemical, nanomaterials and pharmaceutical engineering (See Yan et al. [1], Gao et al. [2-3], Gao and Farahani [4-5], Gao and Shi [6], and Gao and Wang [7-10] for more detail). The referred notations and terminologies without clear explanations can be found in Bondy and Mutry [11].

Furtula et al. [12] defined the generalized version of the atom-bond connectivity index which was defined as:

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$$ABC_\lambda(G)=\sum_{uv\in E(G)}\left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)^{-\lambda},$$

where $\lambda<0$. Clearly, taking $\lambda=-\frac{1}{2}$, it becomes the atom-bond connectivity index defined by Estrada et al. [13]. Also, Furtula et al. [12] introduced the augmented Zagreb index which was denoted as:

$$AZI(G)=\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^{3}.$$

Obviously, the augmented Zagreb index is a special case of the generalized atom-bond connectivity index when $\lambda=3$.

Despite the contributions to the distance-based indices and degree-based molecular structures, the researches of the generalized atom-bond connectivity index for certain special drug structures still await further studies. As a consequence, the research on the generalized atom-bond connectivity index of the drug molecular structure from a mathematical point of view are becoming more and more heated with the years with more and more academic and industrial interest drawn from a variety of fields.

Respectively, we designate $\delta(G)$ and $\Delta(G)$ to be the minimum and maximum degrees of *G*. The edge set *E*(*G*) can be categorized into different parts: for any *i* and *j*, $\delta(G)\le i,j\le\Delta(G)$, let E_{ij} = {e=*uv* ∈ *E*(*G*)| $d(v)=i$, $d(u)=j$} and $n_{ij}=\left|E_{ij}\right|$.

In this paper, we obtain the generalized atom-bond connectivity index of several important chemical structures with a high frequency in drug structures.

MAIN RESULTS

The generalized atom-bond connectivity index of graphene $G(m,n)$

Graphene, a two-dimensional material, is a planar sheet of carbon atoms. It is usually densely packed in a honeycomb crystal lattice and also the main element of certain carbon allotropes including charcoal, fullerenes and graphite, please refer to Figure 1.

Theorem 1. Let $G(m,n)$ be a graphene sheet with *n* rows and *m* columns. We obtain:

$$ABC_\lambda(G(m,n))=$$
$$\begin{cases}(4m+3n)(\frac{1}{2})^{-\lambda}+(\left\lceil\frac{n}{2}\right\rceil(5m+1)+\left\lfloor\frac{n}{2}\right\rfloor(m+3))(\frac{4}{9})^{-\lambda}, & n\equiv 1(\bmod 2)\\ (4m+3n)(\frac{1}{2})^{-\lambda}+(\left\lceil\frac{n}{2}\right\rceil(5m+1)+\left\lfloor\frac{n}{2}\right\rfloor(m+3)+2m-1)(\frac{4}{9})^{-\lambda}, & n\equiv 0(\bmod 2)\end{cases}.$$

Proof. Based on the structure analysis, we obtain:

$$\left|E(G(m,n))\right| = \begin{cases}\left\lceil\frac{n}{2}\right\rceil(5m+1)+\left\lfloor\frac{n}{2}\right\rfloor(m+3), & n\equiv 1(\bmod 2)\\ \left\lceil\frac{n}{2}\right\rceil(5m+1)+\left\lfloor\frac{n}{2}\right\rfloor(m+3)+2m-1, & n\equiv 0(\bmod 2)\end{cases}$$

After further calculation, we get $n_{22}=n+4$, $n_{23}=4m+2n-4$, and

$n_{33}=\left|E(G(m,n))\right|-4m-3n$.

As a result, according to the definition of the generalized atom-bond connectivity index, we obtain the expected result.

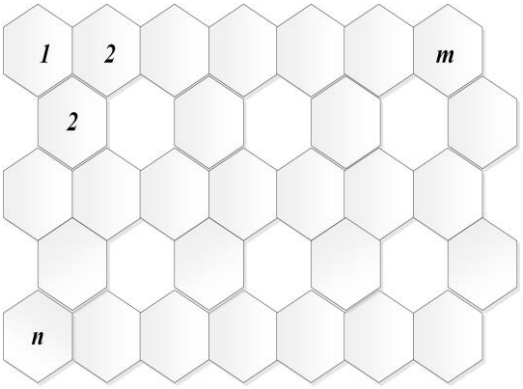

Fig. 1. 2-Dimensional graph of a graphene sheet

Generalized atom-bond connectivity index of three family of dendrimer stars

In this section, three famous infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ of dendrimer stars are defined and they are common in the drug structures.

Theorem 2. Let *n* be the number of steps of growth in this type of dendrimer stars. We indicate

$$ABC_\lambda(NS_1[n])=(27\cdot 2^n-9)(\frac{1}{2})^{-\lambda}+(\frac{2}{3})^{-\lambda}+3(\frac{5}{12})^{-\lambda},$$

$$ABC_\lambda(NS_2[n])=(36\cdot 2^n-6)(\frac{1}{2})^{-\lambda}+(\frac{4}{9})^{-\lambda},$$

$$ABC_\lambda(NS_3[n])=(50\cdot 2^n-13)(\frac{1}{2})^{-\lambda}+2^{n+1}(\frac{2}{3})^{-\lambda}+6\cdot 2^n(\frac{4}{9})^{-\lambda}.$$

Proof. After the observation to the structures

of these three dendrimer stars, we present its edge dividing below:

- for $NS_1[n]$: $n_{23} = 18 \cdot 2^n - 12$, $n_{22} = 9 \cdot 2^n + 3$, $n_{13} = 1$ and $n_{34} = 3$;
- for $NS_2[n]$: $n_{23} = 24 \cdot 2^n - 8$, $n_{22} = 12 \cdot 2^n + 2$ and $n_{33} = 1$;
- for $NS_3[n]$: $n_{23} = 28 \cdot 2^n - 6$, $n_{22} = 22 \cdot 2^n - 7$, $n_{33} = 6 \cdot 2^n$ and $n_{13} = 2^{n+1}$.

Hence, with the reference to the definition of the generalized atom-bond connectivity index, we obtain the expected result.

Generalized atom-bond connectivity index of polyomino chains of n-cycles and triangular benzenoid

In the field of mathematics, a polyomino system, an edge-connected union of cells, is a finite 2-connected plane graph where each interior face (i.e. cell) is encircled by a C_4. More details can be found in Klarner [14] and Ghorbani and Ghazi [15]. For instance, the polyomino chains of 8-cycles can be represented in Figure 2.

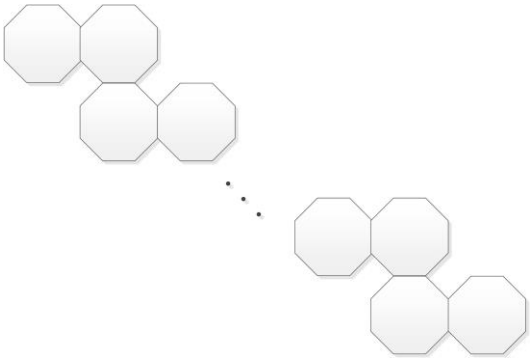

Fig. 2. The zig-zag chain of 8-cycles.

Theorem 3. Let G be a molecular graph as described above. We have

$$ABC_\lambda(G) = (20n+4)(\frac{1}{2})^{-\lambda} + (8n-3)(\frac{4}{9})^{-\lambda}.$$

Proof. Based on the structure analysis, we infer $n_{22} = 12n+4$, $n_{23} = 8n$, and $n_{33} = 8n-3$.

Therefore, considering the definition of the generalized atom-bond connectivity index, we get the expected result.

Next, the generalized atom-bond connectivity index of a triangular benzenoid molecular graph $T(n)$ is computed and the structure is described in Figure 3.

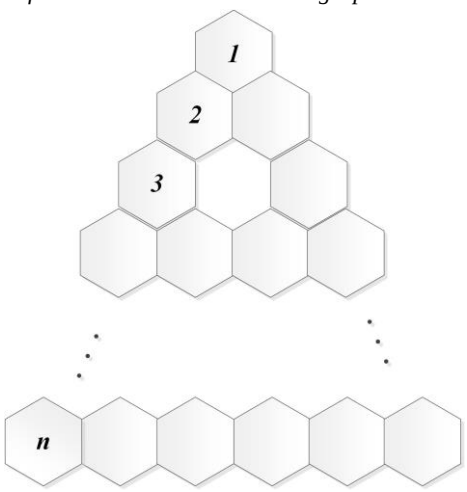

Fig. 3. Molecular graph of a triangular benzenoid $T(n)$

Theorem 4. Let $T(n)$ denote a triangular benzenoid. We get

$$ABC_\lambda(T(n)) = \frac{3n^2-3n+12}{2}(\frac{1}{2})^{-\lambda} + (6n-6)(\frac{4}{9})^{-\lambda}.$$

Proof. Based on the edge dividing technology, we get n_{22} =6, n_{23} = $\frac{3n(n-1)}{2}$, and n_{33} = $6(n-1)$. Hence, concerning the definition of the generalized atom-bond connectivity index, we obtain the result.

Generalized atom-bond connectivity index of bridge molecular structures

Let's consider $\{G_i\}_{i=1}^d$ a set of finite pairwise disjoint molecular graphs with $v_i \in V(G_i)$. The bridge molecular graph $B(G_1,\cdots,G_d) = B(G_1,\cdots,G_d;v_1,\cdots,v_d)$ of $\{G_i\}_{i=1}^d$ regarding the vertices $\{v_i\}_{i=1}^d$ is aquired from the molecular graphs $G_1,\cdots,G_d$ where the vertices v_i and v_{i+1} are linked through an edge for $i = 1,2,\cdots,d-1$. As a result, this section helps to determine the formulas of some degree based indices for the infinite family of drug structures of the bridge molecular graph with $G_1,\cdots,G_d$ (see Figure 4). Then we define $G_d(H,v) = B(H,\cdots,H,v,\cdots,v)$ for special situations of the bridge molecular graphs.

We analyze the bridge graphs as follows and the main parts of the graphs are path, cycle and complete molecular graph, respectively.

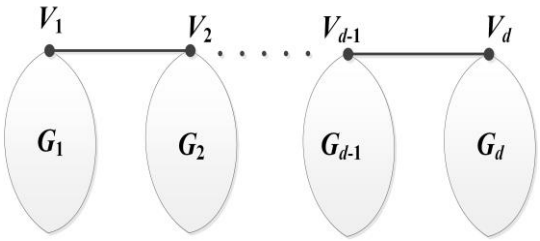

Fig. 4. The bridge molecular graph.

• Let P_n be the path with *n* vertices. We have dn vertices and $dn-1$ edges for the bridge molecular graph $G_d(P_n,v)$ (see Figure 5 for more details). Moreover, the edge set of the bridge graph $G_d(P_n,v)$ can be categorized into four parts: $n_{22}=d(n-3)+2$, $n_{23}=n_{12}=d$, and $n_{33}=d-3$.

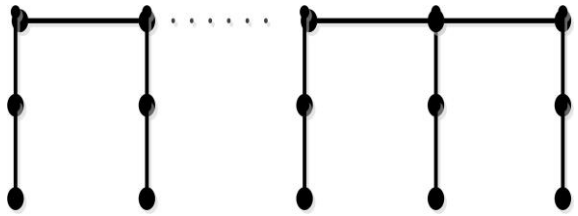

Fig. 5. The bridge molecular graph $G_d(P_n,v)$.

• Let C_n be the cycle with *n* vertices. We get dn vertices and $dn+d-1$ edges for the bridge molecular graph $G_d(C_n,v)$ (see Figure 6 for more details). Moreover, the edge set of the bridge molecular graph $G_d(C_n,v)$ can be categorized into five parts: $n_{22}=d(n-2)$, $n_{23}=4$, $n_{24}=2d-4$, $n_{34}=2$ and $n_{44}=d-3$.

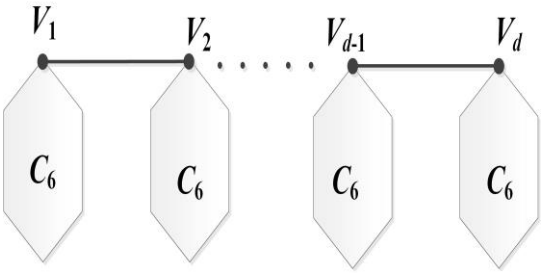

Fig. 6. The bridge molecular graph $G_d(C_n,v)$.

• Let K_n be a complete molecular graph with *n* vertices. We get dn vertices and $\frac{dn(n-1)}{2}+d-1$ edges for the bridge molecular graph $G_d(K_n,v)$ (see Figure 7, $G_d(K_3,v)$ as an example). Moreover, the edge set of the bridge molecular graph $G_d(K_n,v)$ can be categorized into five partitions: $n_{55}=n_{5(n-1)}=d-2$, $n_{45}=n_{4(n-1)}=2$ and $n_{(n-1)(n-1)}=\frac{d(n-1)(n-2)}{3}$.

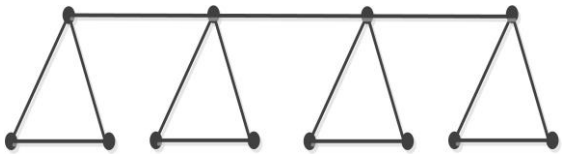

Fig. 7. The bridge molecular graph $G_d(K_3,v)$.

In view of the definition of the generalized atom-bond connectivity index, the main result of this section is obtained and represented below. The detailed proofs are omitted here.

Theorem 5.

$$ABC_\lambda(G_d(P_n,v))=d(n-1)(\frac{1}{2})^{-\lambda}+(d-3)(\frac{4}{9})^{-\lambda},$$

$$ABC_\lambda(G_d(C_n,v))=$$

$$dn(\frac{1}{2})^{-\lambda}+(d-3)(\frac{3}{8})^{-\lambda}+2(\frac{5}{12})^{-\lambda},$$

$$ABC_\lambda(G_d(K_n,v))=(d-2)(\frac{8}{25})^{-\lambda}+2(\frac{7}{20})^{-\lambda}$$

$$+2(\frac{1}{4})^{-\lambda}+(d-2)(\frac{n+2}{5(n-1)})^{-\lambda}$$

$$+\frac{d(n-1)(n-2)}{3}(\frac{2n-4}{(n-1)^2})^{-\lambda}.$$

Generalized atom-bond connectivity index of the carbon tube networks

In this section, we place emphasis on the $m\times n$ quadrilateral section P_m^n with $m\geq 2$ hexagons on the top and bottom sides and $n\geq 2$ hexagons on the lateral sides cut from the regular hexagonal lattice *L*, refer to Figure 8 to observe the detailed chemical structure.

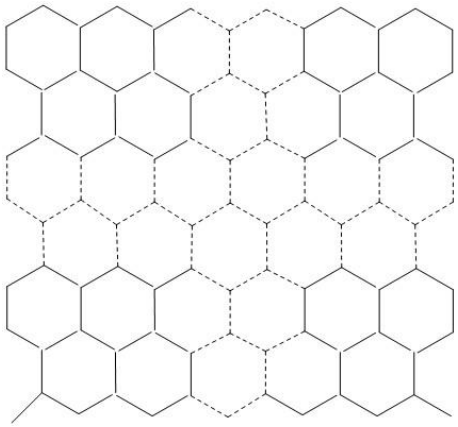

Fig. 8 Quadrilateral section P_m^n cuts from the regular hexagonal lattice.

The tube NA_m^n with $2m(n+1)$ vertices and $(3n+2)m$ edges is obtained by identifying two lateral sides of P_m^n by identifying the vertices u_0^j and u_m^j ($j=0,1,\cdots,n$).

Let $n\in$ be even so that $n,m\geq 2$. The tube NC_m^n of order $n(2m+1)$ with size $n(3m+\frac{1}{2})$ can be obtained if we identify the top and bottom sides of the quadrilateral section P_m^n in a similarly way in which the vertices u_i^0 and u_i^n for $i=0,1,\cdots,m$ and vertices v_i^0 and v_i^n for $i=0,1,\cdots,m$ are identified. See Baca et al. [16] for more details.

Theorem 6.

$$ABC_\lambda(NA_m^n)=4m(\frac{1}{2})^{-\lambda}+m(3n-2)(\frac{4}{9})^{-\lambda},$$

$$ABC_\lambda(NC_m^n)=3n(\frac{1}{2})^{-\lambda}+n(3m-\frac{5}{2})(\frac{4}{9})^{-\lambda}.$$

Proof. For tube NA_m^n, we derive $n_{23}=4m$, and $n_{33}=m(3n-2)$. For tube NC_m^n, we derive $n_{22}=n$, $n_{23}=2n$, and $n_{33}=n(3m-\frac{5}{2})$. Hence, in accordance with the definition of the for the generalized atom-bond connectivity index, we obtain the desired result.

Generalized atom-bond connectivity index of dendrimer stars $D_3[n]$

In this section, an essential chemical structure $D_3[n]$ is analyzed. It describes the *n*-th growth of star dendrimer for $\forall n\in N\cup\{0\}$. Refer to Figure 9 for more details on the structure of this chemical molecular graph which is quite common in drug structures.

Based on the analysis in Farahani [17], we know that $E(D_3[n])$ can be divided into four parts: $n_{13}=3\cdot 2^n$, $n_{22}=6(2^{n+1}-1)$, $n_{23}=12(2^{n+1}-1)$, and $n_{33}=9\cdot 2^n-6$. Hence, we get the conclusion described below for these molecular structures.

Theorem 7. $ABC_\lambda(D_3[n])=3\cdot 2^n(\frac{2}{3})^{-\lambda}$

$$+18(2^{n+1}-1)(\frac{1}{2})^{-\lambda}+(9\cdot 2^n-6)(\frac{4}{9})^{-\lambda}.$$

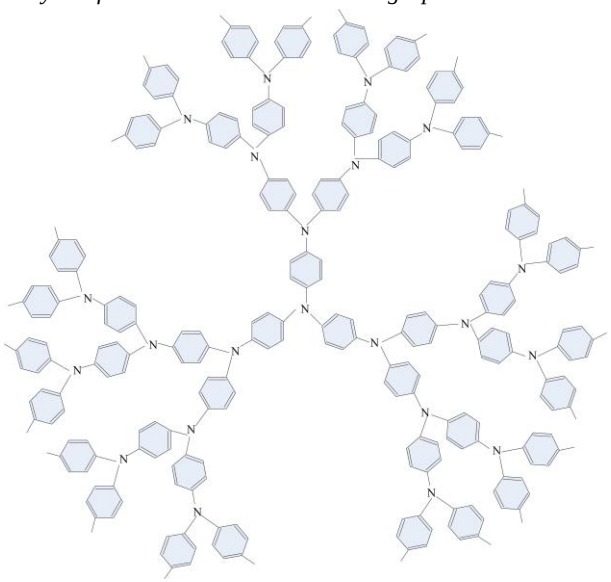

Fig. 9. The 2-Dimensional of the *n*-th growth of star dendrimer $D_3[n]$.

Generalized atom-bond connectivity index of two classes of benzenoid series

In this section, we plan to determine the generalized atom-bond connectivity index of two classes of benzenoid series.

First, the circumcoronene series of benzenoid H_k is concerned. While *k*=1, 2, 3, the structures are presented in Figure 10.

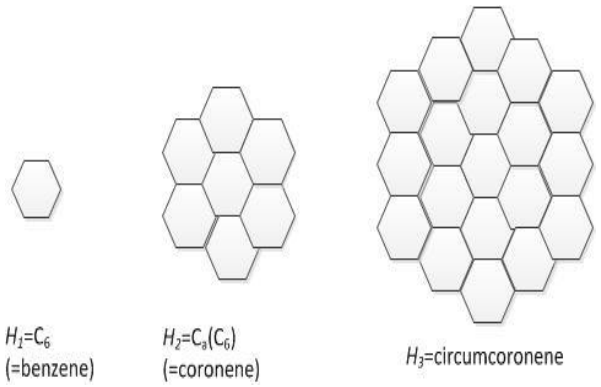

Fig. 10. The first, second and third molecular graphs H_1, H_2 and H_3 from the circumcoronene series of benzenoid.

Hence, the family of circumcoronene homologous series of benzenoid is made up of some copies of benzene C_6 on circumference, for more details of this structure, please refer to Figure 11.

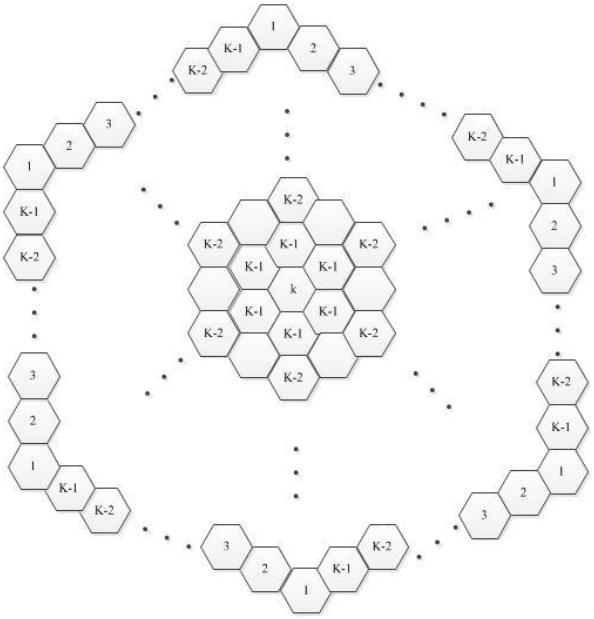

Fig. 11. The circumcoronene series of benzenoid H_k for $k \geq 1$.

Theorem 8.

$$ABC_\lambda(H_k) = (12k-6)(\frac{1}{2})^{-\lambda} + (9k^2-15k+6)(\frac{4}{9})^{-\lambda}.$$

Proof. Consider the circumcoronene series of benzenoid H_k for $k \geq 1$. It is not hard to check that $|V(H_k)| = 6k^2$ and $|E(H_k)| = 9k^2-3k$. Moreover, we deduce $n_{33} = 9k^2-15k+6$, $n_{23} = 12(k-1)$, and $n_{22} = 6$. Thus, regarding the definition of the generalized atom-bond connectivity index, we indicate the result.

Next, the capra-designed planar benzenoid series $Ca_k(C_6)$ (the structure can be referred to Farahani and Vlad [18] for more details) is considered. By means of the intermediate results presented in Farahani and Vlad [18], we present the generalized atom-bond connectivity index of $Ca_k(C_6)$ which is stated as follows.

Theorem 9. $ABC_\lambda(Ca_k(C_6)) = (5\cdot 3^k+3)(\frac{1}{2})^{-\lambda} + (3\cdot 7^k - 2\cdot 3^k - 3)(\frac{4}{9})^{-\lambda}$.

Proof. Based on the analysis of the molecular structure of $Ca_k(C_6)$, we check that the edge set of $Ca_k(C_6)$ can be divided into three partitions: $n_{22} = 3^k+3$, $n_{23} = 4\cdot 3^k$, and $n_{33} = 3\cdot 7^k - 2\cdot 3^k - 3$. Thus, using the definition of the generalized atom-bond connectivity index, we infer the desired result.

OTHER CONCLUSIONS

Finally, we present the generalized atom-bond connectivity index for the chemical structures discussed in Gao et al. [2].

Theorem 10. Let $SP[n]$ be the Dox-loaded micelle comprising a PEG-PAsp block copolymer with a chemically conjugated Dox. We obtain

$$ABC_\lambda(SP[n]) = (27n+4)(\frac{1}{2})^{-\lambda} + (9n+1)(\frac{2}{3})^{-\lambda} + n(\frac{3}{4})^{-\lambda} + 16n(\frac{4}{9})^{-\lambda} + n(\frac{5}{12})^{-\lambda}.$$

Theorem 11. Let $D_2[n]$ and $D_4[n]$ be polyphenylene dendrimers with *n* stages. We have

$$ABC_\lambda(D_2[n]) = (104\cdot 2^n - 92)(\frac{1}{2})^{-\lambda} + (36\cdot 2^n - 35)(\frac{4}{9})^{-\lambda},$$

$$ABC_\lambda(D_4[n]) = (104\cdot 2^n - 80)(\frac{1}{2})^{-\lambda} + (36\cdot 2^n - 36)(\frac{4}{9})^{-\lambda} + 4(\frac{5}{12})^{-\lambda}.$$

Theorem 12. Let *S* be a benzenoid system with *n* vertices, *h* hexagons and *r* inlets. We infer

$$ABC_\lambda(S) = (n-2h+r+2)(\frac{1}{2})^{-\lambda} + (3h-r-3)(\frac{4}{9})^{-\lambda}.$$

Theorem 13. Let PH be phenylene. We deduce

$$ABC_\lambda(PH) = (2h+r+4)(\frac{1}{2})^{-\lambda} + (6h-r-6)(\frac{4}{9})^{-\lambda}.$$

Theorem 14. Let PAH_n be the Polycyclic Aromatic Hydrocarbons

$$ABC_\lambda(PAH_n) = 6n(\frac{2}{3})^{-\lambda} + (9n^2-3n)(\frac{4}{9})^{-\lambda}.$$

CONCLUSIONS

Accompanied by the contentiously emerging viruses, more and more unnamed diseases are found in the world at a high speed each year. This demands the development of more new drugs to treat them. The generalized atom-bond connectivity index was introduced to measure the medicinal properties of new drugs and it is quite welcome and popular in poor areas. In our paper, based on the detailed drug structure analysis and

edge dividing, we defined the generalized atom-bond connectivity index of certain molecular graphs which frequently appear in drug structures. As a result, the conclusions obtained in our paper show the promising prospects of these applications in pharmacy engineering.

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ОБОБЩЕН АНАЛИЗ НА СВЪРЗАНАТА АТОМНА ВРЪЗКА С НЯКОЛКО МОЛЕКУЛНИ ГРАФИ

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(Резюме)

Много тестове върху лекарства показват силна взаимовръзка между био-медицинските и фармакологичните им характеристики с тяхна молекулна структура. С цел да се подобри възможността на изследователите в медицината и фармацията да оценят характеристиките на нови лекарства е дефиниран обобщен индекс на свързаната атомна връзка за анализа на молекулната структура на лекарствата. В тази работа се предлага обобщен индекс на атомните връзки на няколко известни структури, които са твърде сходни с молекулните графи на лекарствата.