Saudi Pharmaceutical Journal 25 (2017) 548–555

Contents lists available at ScienceDirect

Saudi Pharmaceutical Journal

journal homepage: www.sciencedirect.com

Original article

The first multiplication atom-bond connectivity index of molecular structures in drugs

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ARTICLE INFO

Article history:
Available online 28 April 2017

Keywords:
Theoretical medicine
Molecular graph
Multiplicative atom-bond connectivity index
Dendrimer

ABSTRACT

In the field of medicine, there are a large number of new drugs synthesis every year. Before entering the clinical stage, it needs a lot of work on drug testing of the various properties. Due to the lack of a large number of laboratory technician, laboratory equipment and reagents, the drug testing of many biochemical properties are not completed. Theoretical medicine provides a theoretical way for medical researchers to obtain the pharmaceutical properties of compounds by calculation tricks. In this paper, the first multiplication atom-bond connectivity index of several common drugs structure are studied, and the accurate expressions are determined. These theoretical conclusions provide practical guiding significance for pharmaceutical engineering.

1. Introduction

The increasing emergence of disease and the more and more mature medicine technology stimulate the development of newly invented drugs every year. As a result, it proposed the need to determine the pharmacological, chemical and biological features of these new drugs in experiments (Halim and Phang, 2017). On the other hand, it also threw us the tough work and make the relevant research much more headache. To be detailed, qualified and adequate reagents equipment and assisted researchers are necessary in the measurement for the performances and the side effects of the existing drugs (Mustafa et al., 2017). However, the equipment for the measurement of the biochemical properties is a tough problem in poor areas like some parts in South America, Africa and Southeast Asia. What should be glad is that the connection between chemical and pharmacodynamics characteristics of drugs and their molecular structures is found by researchers before (Feng et al., 2016; Xie et al., 2016; Tao et al., 2016). Concerning the definition of the topological indices, the indicators of these drug molecular structures are calculated. As a result, it's turned out to be efficient to make clear the medicinal properties and it can guarantee the well going of medicine and chemical experiments. In other word, the methods on topological index computation can help to get the available biological and medical information of new drugs without the support of chemical experiment hardware (Liu et al., 2016; Iftakhar et al., 2015; Sarfraz et al., 2016). Consequently, it is proved to be suitable to be used in poor parts of the world.

In the below, let $G = (V(G), E(G))$ be a molecular graph with vertex set $V(G)$ and edge set $E(G)$, then we can look upon a topological index as a map f: $G \to \mathbb{R}^+$. Several degree-based or distance-based indices like Randic index, Wiener index, harmonic index, PI index, sum connectivity index and others are borrowed here. Moreover, there are some mention-able contributions on distance-based and degree-based indices of special molecular structures and they can be referred to Harishchandra and Ramane (2016), Gao et al. (2016a,b,c,d), Gao et al. (2017a), Gao and Siddiqui (2017), Gao and Wang (2015, 2016) and Gao et al. (2017b).

The atom-bond connectivity index (shortly, *ABC* index) is defined by Estrada et al. (1998) as

$$ABC_1(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}.$$

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Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

http://dx.doi.org/10.1016/j.jsps.2017.04.021

Very recently, Kulli (2016) defined the first multiplicative atom-bond connectivity index which stated as

$$ABC_1\mathrm{II}(G) = \prod_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.$$

Many papers contributed to different kinds of atom-bond connectivity indices. Farahani (2013a,b) determined the fourth atom-bond connectivity index of circumcoronene series of benzenoid. Goubko et al. (2015) presented an example to show the contradiction on the main result of previous work. Ahmadi and Sadeghimehr (2010) computed the atom bond connectivity index of some graphs and an infinite class of nanostar dendrimers. Husin et al. (2013) obtained the atom bond connectivity index of two families of nanostar dendrimers. Dehghan-Zadeh and Ashrafi (2014) studied the atom-bond connectivity index of quasi-tree graphs. Dehghan-Zadeh et al. (2014) determined the upper bound of atom-bond connectivity index in the class of tetracyclic graphs. Farahani (2013a,b) yielded the fourth atom-bond connectivity index of V-phenylenic nanotubes and nanotori. Dimitrov (2013) researched the efficient computation trick of trees with smallest atom-bond connectivity index. Ashrafi et al. (2015) raised the upper bound of atom-bond connectivity index of cactus graphs with fixed vertex number. Das et al. (2012) established the Upper bounds and Nordhaus-Gaddum type results for atom bond connectivity index.

The past forty years have witnessed the prosperity of the research on computation of degree-based and distance-based indices for certain special drug molecular structure. Despite the disagreements and conflicts on index computation of molecular graphs, the relevant research has made great progresses, but still leaving space for us to keep forward. Moreover, as widespread and critical drug structures, the applications of alkene, cycloalkenes, dendrimers, benzenoid systems and phenylenes are frequently found in chemical, medical, biological and pharmaceutical engineering. Therefore, a further discussion is needed to calculate the drug structures (Chen et al., 2016; Nawaz et al., 2017; Rashid et al., 2017).

The main contribution in this work is threefold: (1) the first multiplicative atom-bond connectivity index of alkene and cycloalkenes is obtained; (2) the expressions of the first multiplicative atom-bond connectivity index of special dendrimers are raised; (3) the formula of the first multiplicative atom-bond connectivity index of benzenoid systems and phenylenes is also obtained and analyzed.

2. Main results and proofs

In the below, the minimum and maximum degree of G are denoted by $\delta(G)$ and $\Delta(G)$. Edge set $E(G)$ and vertex set $V(G)$ are categorized into the following items:

- for any i with $\delta(G) \leqslant i \leqslant \Delta(G)$, let $D_i = \{u \in V(G) | d(v) = i\}$ and $d_i = |D_i|$
- for any i, j satisfy $\delta(G) lesi$, $j \leqslant \Delta(G)$, let $E_{i,j} = \{e = uv \in E(G) | d(u) = i,$ and $d(v) = j\}$ and $n_{ij} = |E_{i,j}|$.

2.1. The first multiplicative atom-bond connectivity index of alkene and cycloalkenes

In this part, we discuss the structure on alkene and cycloalkenes which are widely used in medicine and pharmaceutical engineering. Some applications on alkene and cycloalkenes can refer to Dziechciejewski et al. (2015), Babaee et al. (2012), Sysoiev et al. (2012), Tsarev et al. (2010), and Wilson et al. (2007).

As an unsaturated hydrocarbon with at least one carbon-carbon double bond, an alkene is composed of two hydrogen atoms less than the relevant alkane which has the same number of carbon atoms, with general formula C_nH_{2n}. The smallest alkene is ethylene (C_2H_4). Only a dobell bond between any two atoms of carbon is used to build the multiplicative ABC index for alkene, and in the

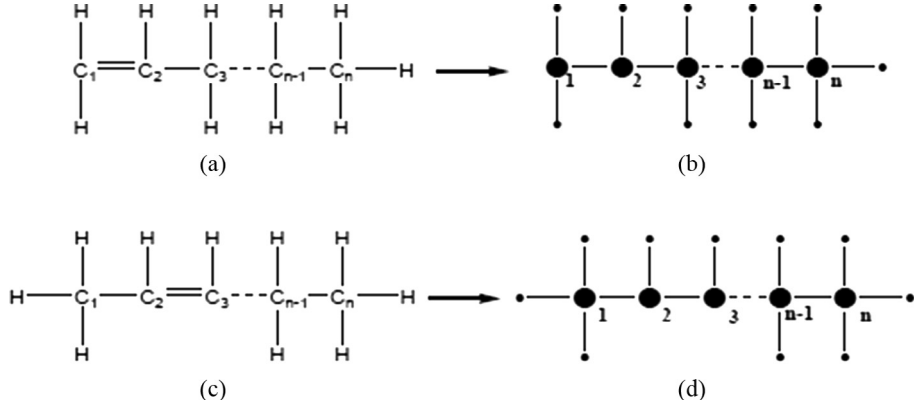

Fig. 1. (a) and (c) denote the molecular structure of alkenes C_nH_{2n}; (b) and (d) denote the molecular graph associated with chemical compound of alkenes C_nH_{2n}.

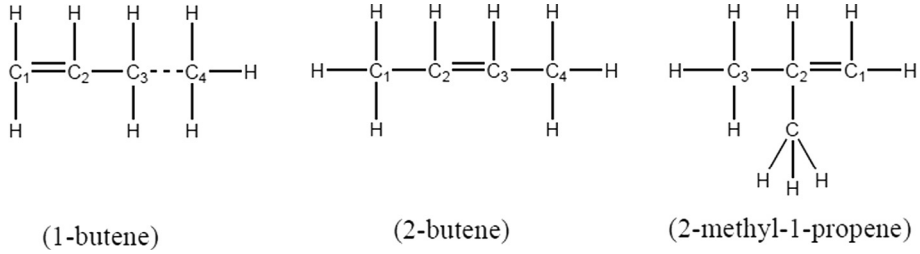

Fig. 2. Molecular structure of butene and methylpropene.