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2-求和连通指数的研究

阿耶莎·赛义德·巴蒂
（政府学院大学 数学系，拉合尔 54000）

摘要：透明质酸-紫杉醇（HA-PTX）也称为透明质酸（HA），是天然存在的化合物. 其是一种由 D-葡萄糖醛酸和 N-乙酰基-D-葡萄糖胺单元的线性结构组成的糖胺聚糖聚合物，它们通过交替的-1，3-和-1，4-糖苷键连接. 在化学图论中，将图关联到化合物并计算拓扑指数，有助于猜测未充分研究的化合物的性质. 因此，计算了 2-求和连接性指数，例如，2-求和原子健连通指数、2-求和逆 Randic 指数、2-求和几何算术指数、2-求和第 1 重定义的 Zagreb 指数、2-求和第 2 重定义的 Zagreb 指数、HA - PTX 的 2-求和第 3 重定义的 Zagreb 指数.

关键词：拓扑指数；2 - 求和连通指数；分子图；度
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On 2-sum Connectivity Indices

AYESHA Saeed Bhatti
(Department of Mathematics, Government College University, Lahore, Pakistan　54000)

Abstract: Hyaluronic Acid-Paclitaxel (HA-PTX) also known as Hyaluronic Acid (HA) is a compound that occurs naturally. It is a glycosaminoglycan polymer composed of a linear structure of units of D-glucuronic acid and N-acetyl-D-glucosamine, which are linked via alternating -1, 3- and -1, 4-glycosidic bonds. In chemical graph theory we associate a graph to a compound and compute topological indices that help us in guessing properties of understudy compound. So we concentrate to compute two sum connectivity indices such as 2-sum atomic bound connectivity index, 2-sum inverse Randic index, 2-sum geometric arithmetic index, 2-sum and first redefined Zagreb index, 2-sum and second redefined Zagreb index, 2-sum and third redefined Zagreb index for HA-PTX.

Key words: topological index; 2-sum connectivity index; molecular graph; degree

0　Introduction

The description of an atomic structure by a graph where the vertices are represented by atoms and the edges are represented by the bonding, is a significant application of (connected undirected) graphs, studied in a field called chemical graph theory.

A molecular graph $G = (V, E)$ is a simple graph having $n = |V|$ vertices and $m = |E|$ edges. The vertices $v_i \in V$ represent non-hydrogen atoms and the edges $(v_i, v_j) \in E$ represent covalent bonds among the corresponding atoms. Hydrocarbons are made up of only carbon and hydrogen atoms and their molecular graphs are represented by the carbon skeleton of the molecule.

Topological indices possibly viewed as a huge variety of boundaries on a subatomic graph that is significant in theoretic physical science and pharmacology science[1-3]. There are some significant indices obsessed on the vertex degree, for example, Randic indices, harmonic index, Zagreb indices etc. The known Randic, has been utilized successfully as an atomic descriptor in QSPR and QSAR[4-5]. In this paper, we defined following 2-sum indices.

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作者简介：阿耶莎·赛义德·巴蒂，女，巴基斯坦人，博士研究生，主要从事图论和组合数学研究.

The 2-sum atomic bound connectivity index is defined as:

$$ABC^2(G) = \sum_{\{i,j,k\} \in p_2} \sqrt{\frac{d_i + d_j + d_k - 2}{d_i \times d_j \times d_k}} .$$

The 2-sum inverse Randic index is defined as:

$$R^2(G) = \sum_{\{i,j,k\} \in p_2} \frac{1}{\sqrt{d_i \times d_j \times d_k}} .$$

The Redefined Zagreb indices are as follows:

$$\mathrm{Re}\, ZG_1^2(G) = \sum_{p^2 = \{i,j,k\} \subseteq E(G)} \frac{(d_i + d_j + d_k)}{(d_i \times d_j \times d_k)};$$

$$\mathrm{Re}\, ZG_2^2(G) = \sum_{p^2 = \{i,j,k\} \subseteq E(G)} \frac{(d_i \times d_j \times d_k)}{(d_i + d_j + d_k)};$$

$$\mathrm{Re}\, ZG_3^2(G) = \sum_{p^2 = \{i,j,k\} \subseteq E(G)} (d_i \times d_j \times d_k)(d_i + d_j + d_k).$$

1 Methodology

To figure our results, firstly we will construct the graph of involved molecular compounds and count the overall range of vertices and edges. Secondly, we tend to divide the edge set of involved graphs into totally different class supported the degrees of end vertices. By applying definitions of 2-sum Atomic Bound connectivity index, 2-sum Inverse Randic index, 2-sum First Redefined Zagreb index, 2-sum Second Redefined Zagreb index, 2-sum Third Redefined Zagreb index for some connectivity indices, we have a tendency to compute our desired results.

2 Hyaluronic Acid-Paclitaxel Conjugates

Threat is seen as one of the noteworthy explanations behind death on the planet and its end extent continues rising with the greater part of passing's achieved by chest, stomach, lung, and colon threatening growths. Regardless of the way that there have been unprecedented enhancements in threatening development science and medicines to treat tumors, challenges notwithstanding everything remain in fundamental and metastatic ailment treatment. Additionally, there are traps in current anticancer drugs which incite low identity and high destructiveness as such genuinely restricting their feasibility. Certain advances have happened in molecularly centered around sickness treatment over late years. Hyaluronic destructive (HA) is a fuel which occurs regularly. It is a glycosaminoglycan polymer made of a straight structure of units of D-glucuronic destructive and N-acetyl-D-glucosamine, which are associated by implies of pivoting -1, 3-and-1, 4-glycosidic bonds. Its fundamental structure, disaccharide, is energetically consistent. HA is a encouraging ailment sedate on account of its novel, biodegradable, bio-feasible, non-toxic, hydrophilic, likewise, non-immutable features; besides, HA receptors showed over-verbalization on various tumor cells. As a rapidly creating stage for zeroing in on CD44-over imparting cells these days, HA intends to improve anticancer therapies. HA is an ideal medicine carrier and prescription zeroing in on. Paclitaxel (PTX) is a convincing medicine, which is proposed for certain sorts of tumors, including ovarian, chest, lung, bladder, prostate, and esophageal tumors, etc. Whereas PTX association furthermore experience its own obstacles, for instance, its powerless dissolvability furthermore, appropriate indications, similarly as the excipients usually used in its arrangement. Ringsdorf at first suggested the procedure for making polymeric macromolecule-sedate structures, which was expected to pass on minimal hydrophobic drug particles to their objections of movement. The crucial good conditions of HA-PTX structures are the development of its water dissolvability and the protecting of its development, most significantly, it could be consumed as engaged medicine movement to strengthen unfriendly to tumor ampleness. The formation of hyaluronic acid-paclitaxel (HA-PTX) structures is represented in Figures 1-3.

For Hyaluronic Acid-Paclitaxel conjugates (HA-PTX $[n]$), we have

$|p\{1, 2, 3\}| = n+1$, $|p\{1, 3, 3\}| = 12n$, $|p\{1, 3, 2\}| = 10n+1$, $|p\{1, 4, 4\}| = 3n$,

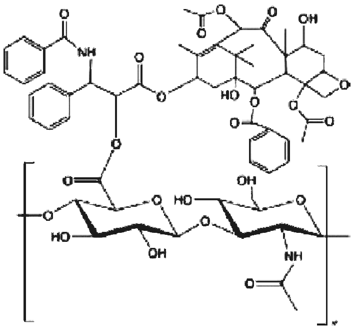

Figure 1　Unit Structure

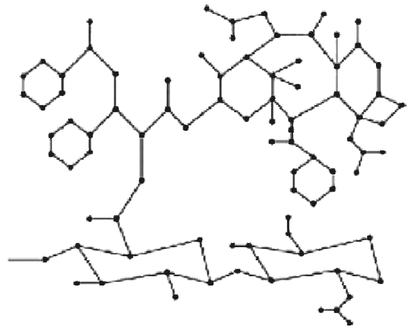

Figure 2　Molecular Graph

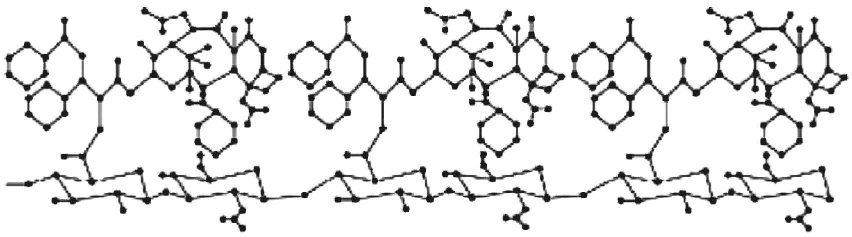

Figure 3　Growth of Graph

$|p\{1,4,3\}|=6n$, $|p\{1,3,4\}|=2n$, $|p\{1,4,1\}|=n$, $|p\{1,4,2\}|=n$, $|p\{1,3,1\}|=3n$, $|p\{2,2,2\}|=9n$, $|p\{2,3,2\}|=8n$, $|p\{2,4,2\}|=n$, $|p\{2,4,3\}|=3n$, $|p\{2,4,4\}|=n$, $|p\{2,3,4\}|=4n$, $|p\{2,3,3\}|=29n$, $|p\{3,3,3\}|=11n$, $|p\{3,4,4\}|=2n$, $|p\{3,4,3\}|=3n$, $|p\{3,2,3\}|=10n-1$, $|p\{3,2,2\}|=9n$, $|p\{4,3,4\}|=n$, $|p\{4,2,3\}|=2n$, $|p\{4,3,3\}|=6n$.

Theorem 1　Let G be the molecular graph of Hyaluronic Acid-Paclitaxel conjugates (HA-PTX), then the 2-sum atomic bound connectivity index is

$$ABC^2(G) = 87.3271n + 1.0557.$$

Proof　By the definition of the 2-sum atomic bound connectivity index, we have

$$\begin{aligned}ABC^2(G) &= \sum_{\{i,j,k\}\in p_2}\sqrt{\frac{d_i+d_j+d_k-2}{d_i\times d_j\times d_k}}\\ &=0.8165n+0.8165+8.9443n+8.1650n+0.8165+1.9843n+4.2426n\\ &+1.4142n+n+0.7906n+3n+6.3640n+5.1640n+0.1624n+1.6202n\\ &+0.5n+2.1602n+16.7431n+5.6010n+0.8660n+1.4142n+5.7735n\\ &-0.5774+5.8095n+0.4330n+1.0801n+2.8284n\\ &=87.3271n+1.0557.\end{aligned}$$

Theorem 2　Let G be the molecular graph of Hyaluronic Acid-Paclitaxel conjugates (HA-PTX), then the 2-sum inverse Randic index is

$$R^2(G) = 34.2742n + 0.5807.$$

Proof　By the definition of the 2-sum inverse Randic index, we have

$$\begin{aligned}R^2(G) &= \sum_{\{i,j,k\}\in p_2}\frac{1}{\sqrt{d_i\times d_j\times d_k}}\\ &= 0.4082n + 0.4082 + 4n + 0.625n + 0.4082 + 0.75n + 1.7321n + 0.5774n + 0.5n\\ &+ 0.3536n + 1.7321n + 3.1820n + 2.3094n + 0.25n + 0.6124n + 0.1768n + 0.8165n\\ &+ 6.8354n + 2.1170n + 0.2887n + 0.5n + 2.3570n - 0.2357 + 2.5981n + 0.1443n\\ &+ 0.4082n + n = 34.2742n + 0.5807.\end{aligned}$$

Theorem 3　Let G be the molecular graph of Hyaluronic Acid-Paclitaxel conjugates (HA-PTX), then the 2-sum first redefined Zagreb index is

$$RZ_1^2(G) = 79.7708n + 1.5556.$$

Proof By the definition of the 2-sum first redefined Zagreb index, we have

$$RZ_1^2(G) = \sum_{\{i,j,k\} \in p_2} \frac{d_i + d_j + d_k}{d_i \times d_j \times d_k}$$
$$= n + 1 + 9.3333n + 10n + 1 + 1.6875n + 4n + 1.3333n + 1.5n + 0.875n + 5n + 6.75n$$
$$+ 4.6667n + 0.5n + 1.125n + 0.3125n + 1.5n + 12.8889n + 3.6667n + 0.4583n$$
$$+ 0.8333n + 4.4444n - 0.4444 + 5.25n + 0.2292n + 0.75n + 1.6667n$$
$$= 79.7708n + 1.5556.$$

Theorem 4 Let G be the molecular graph of Hyaluronic Acid-Paclitaxel conjugates (HA-PTX), then the 2-sum second redefined Zagreb Index is

$$RZ_2^2(G) = 283.9553n - 0.25.$$

Proof By the definition of the 2-sum second redefined Zagreb index, we have

$$RZ_2^2(G) = \sum_{\{i,j,k\} \in p_2} \frac{d_i \times d_j \times d_k}{d_i + d_j + d_k}$$
$$= n + 1 + 15.4286n + 10n + 1 + 5.3333n + 9n + 3n + 0.6667n + 1.1429n + 1.8n$$
$$+ 12n + 3.7143n + 2n + 8n + 3.2n + 10.6667n + 65.25n + 33n + 8.7273n + 10.8n$$
$$+ 22.5n - 2.25 + 15.4286n + 4.3636n + 5.3333n + 21.6n$$
$$= 283.9553n - 0.25.$$

Theorem 5 Let G be the molecular graph of Hyaluronic Acid-Paclitaxel conjugates (HA-PTX), then the 2-sum third redefined Zagreb index is

$$RZ_3^2(G) = 19\,842n - 72.$$

Proof By definition of the 2-sum third redefined Zagreb index, we have

$$RZ_3^3(G) = \sum_{\{i,j,k\} \in p_2} (d_i \times d_j \times d_k)(d_i + d_j + d_k)$$
$$= 36n + 36 + 756n + 360n + 36 + 432n + 576n + 192n + 24n + 56n + 45n + 432n + 672n$$
$$+ 128n + 648n + 320n + 864n + 4\,176n + 2\,673n + 1\,056n + 1\,080n + 1\,440n - 144 + 756n$$
$$+ 528n + 432n + 2\,160n$$
$$= 19\,842n - 72.$$

3 Conclusions

Topological indices can help to solve many problems of chemistry with using lab. In this paper, we introduced concept of 2-sum connectivity indices. We defined 2-sum inverse Randic index, 2-sum atomic bound connectivity index and 2-sum redefined first, second and third Zagreb indices. We also computed aforementioned indices for the molecular graph of Hyaluronic Acid-Paclitaxel conjugates (HA-PTX).

[参考文献]

[1] HOSOYA H. Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons [J]. Bulletin of the Chemical Society of Japan, 1971, 44 (9): 2332 – 2339.

[2] GUTMAN I. Selected properties of the Schultz molecular topological index [J]. Journal of Chemical Information and Computer Sciences, 1994, 34 (5): 1087 – 1089.

[3] GAO W, FARAHANI M R, SHI L. Forgotten topological index of some drug structures [J]. Acta Medica Mediterranea, 2016, 32 (1): 579 – 585.

[4] GAO W, WANG W, DIMITROV D, et al. Nano properties analysis via fourth multiplicative ABC indicator calculating [J]. Arabian Journal of Chemistry, 2018, 11 (6): 793 – 801.

[5] KWUN Y C, MUNIR M, NAZEER W, et al. M-Polynomials and topological indices of V-Phenylenic Nanotubes and Nanotori [J]. Scientific Reports, 2017, 7 (1): 1 – 9.