COMPUTING SOME TOPOLOGICAL INDICES OF SMART POLYMER

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A topological index of a graph *G* is a numeric quantity related to *G* which is describe molecular graph *G*. The Smart polymers are macro-molecules that display a dramatic physiochemical change in response to small changes in their environment such as temperature, pH, light, magnetic field, ionic factors etc. In this paper we compute Randić index, Zagreb index, Geometric-arithmetic index GA and ABC indices of class of smart polymer is computed.

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1. Introduction

Smart polymers are defined as the macromolecules that display a dramatic physiochemical change in response to small changes in their environment such as temperature, pH, light, magnetic field, ionic factors, etc [15]. Smart polymers are also called as stimuli responsive or intelligent or environmentally responsive systems. Smart polymers have various applications in biomedical field as delivery systems like smart polymers with protein or nucleic acid delivery to intracellular targets such as ribosome or nucleus and in tissue engineering [11, 14]. Polymeric micelles are one of the kind of smart polymer, which is used to delivering anti cancer drug. For eg. Dox-conjugated PEG-b-poly (aspartate) (PEG--PAsp) block copolymers [5].

Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of the molecule. Therefore, the topological analysis of a molecule involves translating its molecular structure into a characteristic unique number (or index) that may be considered a descriptor of the molecule under examination. Such indices based on the distances in graph are widely used for establishing relationships between the structure of molecular graph and their physicochemical properties.

Let G be a simple graph, the vertex-set and edge-set of which are represented by $V(G)$ and $E(G)$ respectively. Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [3]. They are defined as:

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$$M_1\,(G) = \sum d(u)^2 \ and \ M_2\,(G) = \sum d(u)d(v), \qquad uv \in E(G),$$
where $d(u)$ and $d(u)$ are the degree of u and v.

The connectivity index introduced in 1975 by Milan Randić [12], who has shown this index to reflect molecular branching. Randic index was defined as follows:

$$\chi(\mathrm{G}) = \sum \frac{1}{\sqrt{d(u)d(v)}},\ uv \in E(G).$$

Another topological index namely, *Geometric-arithmetic index*, (GA index) defined by Vukicević and Furtula [16] as follows:

$$GA(G) = \sum \frac{2\sqrt{\mathrm{d_u d_v}}}{\mathrm{d_u + d_v}}, uv \in E(G).$$

Recently Ernesto Estrada et al. [2], introduced *atom-bond connectivity (ABC) index*, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

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

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. The simplest topological indices do not recognize double bonds and atom types (C, N, O etc.) and ignore hydrogen atoms ("hydrogen suppressed") and defined for connected undirected molecular graphs only [6]. In this paper, we compute these indices [1, 4, 7, 8, 9, 10, 13, 17, 18, 19], for the class of the smart polymer *Dox-loaded micelle comprising PEG-PA*sp block copolymer with chemically conjugated Dox (Fig. 1).

Topological indices for Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox SP[n]

Consider a molecular graph $G(n) = SP[n]$, where n is step of growth of this type of polymers, see Fig. 1 and graph for the $G(1)$, $G(2)$ and $G(3)$, are shown in the fig. 2, fig. 3 and fig. 4 respectively. Define e_{ij} to be the edges connecting vertex of degree i with vertex of degree j.

Using simple calculation we can show that, in $G(n)$ there are 8 types of edges, i.e the edges e_{12}, e_{13} , e_{i4}, e_{22} , e_{23} , e_{24}, e_{33} and e_{34}. There are $2n + 1$ edges of type e_{12} , $9n + 1$ edges of type e_{13}, n edges of type e_{14} and e_{34}, $(5n + 4)$ edges of type e_{22}, $(18\mathrm{n} - 1)$ edges of type e_{23}, $(2\mathrm{n})$ edges of type e_{24} and $16\mathrm{n}$ edges of type e_{33} and the cardinality of the vertex set of $\mathrm{G(n)}$ is $49\mathrm{n} + 6$ and that of the edge set is $(54n + 5)$.

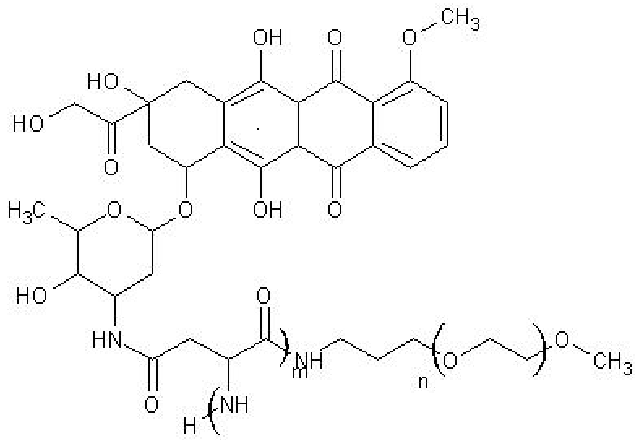

Fig. 1. Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox SP[n] = G(n)

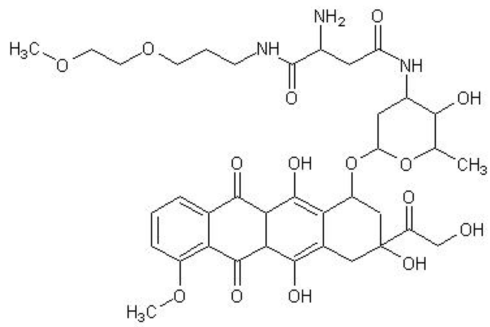

Fig. 2. Graph of G(1)

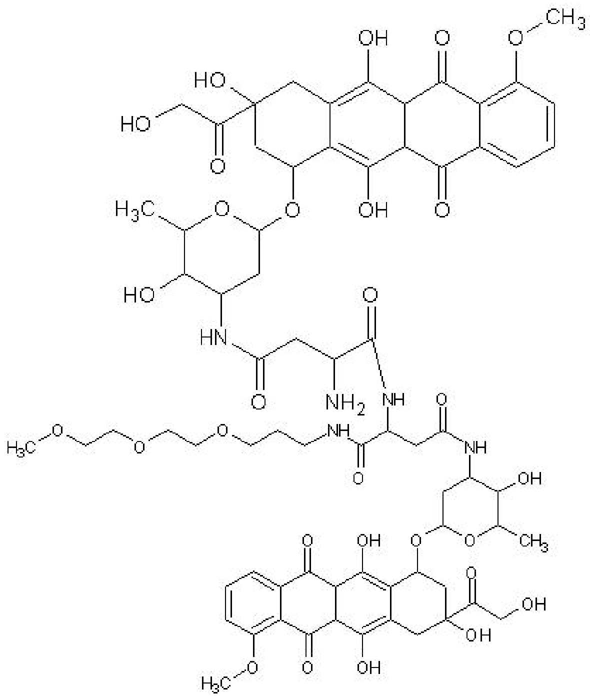

Fig. 3. Graph of G(2)

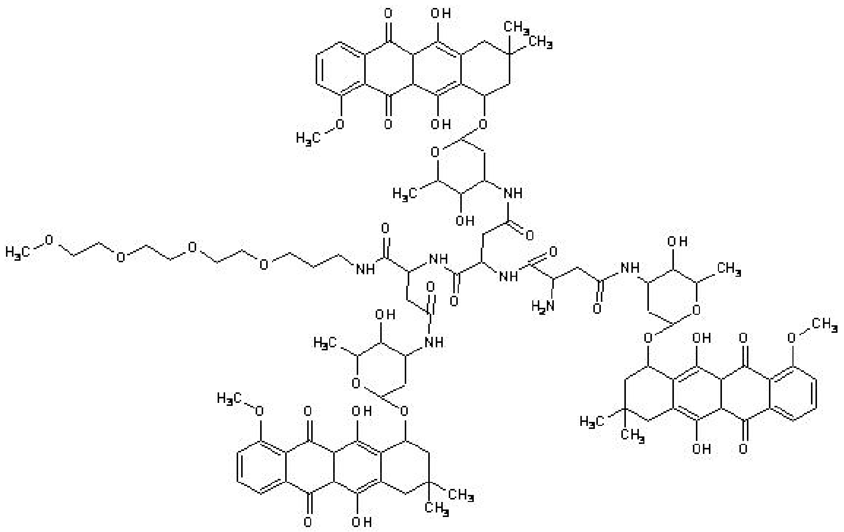

Fig 4. Graph of G(3)

Theorem 1. The Randić index of $G(n)$ is,

$$\chi(G(n)) = \frac{1}{15125898}\,[43505240.3972 + 352251163.892n]$$

Proof: $\chi(G(n)) = \sum_{uv\in e_{12}} \frac{1}{\sqrt{2}} + \sum_{uv\in e_{13}} \frac{1}{\sqrt{3}} + \sum_{uv\in e_{14}} \frac{1}{\sqrt{4}} + \sum_{uv\in e_{22}} \frac{1}{\sqrt{4}} + \sum_{uv\in e_{23}} \frac{1}{\sqrt{6}} + \sum_{uv\in e_{24}} \frac{1}{\sqrt{8}} + \sum_{uv\in e_{33}} \frac{1}{\sqrt{9}} + \sum_{uv\in e_{34}} \frac{1}{\sqrt{12}}$

$= (2n+1)\frac{1}{\sqrt{2}} + (9n+1)\frac{1}{\sqrt{3}} + n\frac{1}{\sqrt{4}} + (5n+4)\frac{1}{\sqrt{4}} + (18n-1)\frac{1}{\sqrt{6}} + 2n\frac{1}{\sqrt{8}} + 16n\frac{1}{\sqrt{9}} + n\frac{1}{\sqrt{12}}$

$\chi(G(n)) = \frac{1}{15125898}\,[43505240.3972 + 352251163.892n]$

Theorem 2. The ABC index of $G(n)$ is

$$ABC(G(n)) = 38.618542n + 3.644924.$$

Proof: $ABC(G(n)) = \sum_{uv\in e_{12}} \frac{1}{\sqrt{2}} + \sum_{uv\in e_{13}} \sqrt{\frac{2}{3}} + \sum_{uv\in e_{14}} \frac{\sqrt{3}}{2} + \sum_{uv\in e_{22}} \frac{1}{\sqrt{2}} + \sum_{uv\in e_{23}} \frac{1}{\sqrt{2}} + \sum_{uv\in e_{24}} \frac{1}{\sqrt{2}} + \sum_{uv\in e_{33}} \frac{2}{3} + \sum_{uv\in e_{34}} \frac{\sqrt{5}}{\sqrt{12}}.$

$$= (2n+1)\frac{1}{\sqrt{2}} + (9n+1)\sqrt{\frac{2}{3}} + n\frac{\sqrt{3}}{2} + (5n+4)\frac{1}{\sqrt{2}} + (18n-1)\frac{1}{\sqrt{2}} + 2n\frac{1}{\sqrt{2}} + 16n\frac{2}{3} + n\sqrt{\frac{5}{12}}$$

$= 38.618542n + 3.644924.$

Theorem 3. The GA index of $G(n)$ is

$$GA(G(n)) = 51.991534267n + 4.82903854825$$

Proof: $GA(G(n)) = \sum_{uv\in e_{12}} \frac{2\sqrt{2}}{3} + \sum_{uv\in e_{13}} \frac{2\sqrt{3}}{4} + \sum_{uv\in e_{14}} \frac{2\sqrt{4}}{5} + \sum_{uv\in e_{22}} \frac{2\sqrt{4}}{4} + \sum_{uv\in e_{23}} \frac{2\sqrt{6}}{5} + \sum_{uv\in e_{24}} \frac{2\sqrt{8}}{6} + \sum_{uv\in e_{33}} \frac{2\sqrt{9}}{3} + \sum_{uv\in e_{34}} \frac{2\sqrt{12}}{7}.$

$$= (2n+1)\frac{2\sqrt{2}}{3} + (9n+1)\frac{2\sqrt{3}}{4} + n\frac{2\sqrt{4}}{5} + (5n+4)\frac{2\sqrt{4}}{4} + (18n-1)\frac{2\sqrt{6}}{5} + 2n\frac{2\sqrt{8}}{6} + 16n\frac{2\sqrt{9}}{6} + n\frac{2\sqrt{12}}{7}$$

$= 51.991534267n + 4.82903854825.$

Theorem 4. The $First\ Zagreb$ index of $G(n)$ is

$$M_1\left(G(n)\right) = 272n + 18.$$

Proof: In $G(n)$ there are $(49n+9)$ vertices, among which $(12n+2)$ vertices having degree 1, $(16n+4)$ vertices having degree 2, $20n$ vertices having degree 3 and n vertices having degree 4. Hence,

$$M_1\left(G(n)\right) = (12n+2) + (16n+4)2^2 + 20n\, 3^2 + n\, 4^2$$

$$M_1\left(G(n)\right) = 272n + 18.$$

Theorem 5. The $Second\ Zagreb$ index of $G(n)$ is

$$M_2\left(G(n)\right) = 335n + 15.$$

Proof:

$M_2\left(G(n)\right) = \sum_{uv\in e_{12}} 2 + \sum_{uv\in e_{13}} 3 + \sum_{uv\in e_{14}} 4 + \sum_{uv\in e_{22}} 4 + \sum_{uv\in e_{23}} 6 + \sum_{uv\in e_{24}} 8 + \sum_{uv\in e_{33}} 9 + \sum_{uv\in e_{34}} 12 = 335n + 15.$.

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