Research Article

Open Access

Shazia Manzoor, Yu-Ming Chu*, Muhammad Kamran Siddiqui and Sarfraz Ahmad

On topological aspects of degree based entropy for two carbon nanosheets

<https://doi.org/10.1515/mgmc-2020-0025>

Received July 21, 2020; accepted November 10, 2020.

Abstract: The entropy-based procedures from the configuration of chemical graphs and multifaceted networks, several graph properties have been utilized. For computing, the organizational evidence of organic graphs and multifaceted networks, the graph entropies have converted the information-theoretic magnitudes. The graph entropy portion has attracted the research community due to its potential application in chemistry. In this paper, our input is to reconnoiter graph entropies constructed on innovative information function, which is the quantity of different degree vertices along with the quantity of edges between innumerable degree vertices.”In this study, we explore two dissimilar curricula of carbon nanosheets that composed by C_4 and C_8 denoted by $T^1C_4C_8(S)[m, n]$ and $T^2C_4C_8(R)[m, n]$. Additionally, we calculate entropies of these configurations by creating a connection of degree-based topological indices with the advantage of evidence occupation.

Keywords: entropy; Zagreb kind indices; Balaban index; carbon nanosheets; $T^1C_4C_8(S)[m, n]$; $T^2C_4C_8(R)[m, n]$

1 Introduction

A branch of mathematical chemistry that uses the tools of graph theory to develop the organic phenomenon mathematically is called chemical graph theory (Ali et al., 2019). Additionally, for resolving molecular problems,

chemical graph theory links to the nontrivial solicitations of graph theory. This theory has important applications in the domain of chemical sciences (Gao and Farahani, 2016; Gao et al., 2018). Chem-informatics (containing chemistry and information science) analysis (QSAR) and (QSPR) are used to anticipate the bioactivity and physiochemical possessions of organic mixtures (Wu et al., 2015).

G is a graph in which the vertex and the edge set are represented by $V(G)$ and $E(G)$, respectively. The degree $\Xi(r)$ of a vertex r is the quantity of edges of G contiguous with vertex r . Let G be a graph with m vertices and n edges, where m embodies the order and n refers to the size of the graph. A graph of order m and size n is characterized as (m, n) -graph see: Assaye et al. (2019), Basavanagoud et al. (2017), Hosamani et al. (2017), and Shirakol (2019).

In molecular graph, the vertices designate atoms and edges signpost as the substance bonds. A arithmetic value that is calculated arithmetically by using the molecular graph is characterized as a topological index. It is connected to chemical composition demonstrating for association of chemical structure with plentiful physical, chemical possessions and biological activities. For further details of formulas of topological indices and application points see: Siddiqui et al., (2016a, 2016b), and Gao et al. (2017) and Imran et al. (2018), respectively.

The basic idea of entropy was introduced in the following statement: “The entropy of a possible dissemination is known as a quota of the unpredictability of evidence content or a portion of the uncertainty of a coordination” (Shannon, 2001), which was developed for evaluating the mechanical evidence of graphs and chemical networks.

Afterward, it has been used significantly in graphs and chemical networks. Rashevsky (1955) introduced the graph entropy impression established on the classifications of vertex orbits in 1955. Currently, graph entropies have been widely pragmatic in an extensive assortment of questions, such as chemistry and sociology (Dehmer and Grabner, 2013; Ulanowicz, 2004).

There are many specific categories of aforementioned graph entropy procedures. They associate probability

*Corresponding author: Yu-Ming Chu, Department of Mathematics, Huzhou University, Huzhou 313000, P. R. China; Hunan Provincial Key Laboratory of Mathematical Modeling and Analysis in Engineering, Changsha University of Science & Technology, Changsha 410114, P. R. China; e-mail: chuyuming@zjhu.edu.cn

Shazia Manzoor, Muhammad Kamran Siddiqui and Sarfraz Ahmad, Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Pakistan; e-mail: shazman724@gmail.com, kamransiddiqui75@gmail.com, sarfrazahmad@cuilahore.edu.pk

distributions with elements (vertices, edges, etc.) of a graph that can be categorized as core and extrinsic dealings. Dehmer (2008) and Dehmer et al. (2012) presented information based function graph entropies, which imprisonment operational evidence and analyze their properties. For more details, see: Bonchev (2003), Dehmer and Mowshowitz (2011), Morowitz (1955), Rashevsky (1955), Shannon (2001), Solé and Valverde (2004), Quastler (1954), Tan and Wu (2004), and Trucco (1956).

2 Degree based topological indices of graph

Gutman with coauthors (Gutman and Das, 2004; Gutman and Trinajstić, 1972) defined first and second Zagreb index as:

$$M_1 = \sum_{rs \in E(G)} (\Xi(r) + \Xi(s)), \quad M_2(G) = \sum_{rs \in E(G)} (\Xi(r) \times \Xi(s))$$

Shirdel et al. (2013) introduced “hyper Zagreb index” as:

$$HM = \sum_{rs \in E(G)} (\Xi(r) + \Xi(s))^2$$

Furtula and Gutman (2015) defined F-index as:

$$F(G) = \sum_{rs \in E(G)} \left((\Xi(r))^2 + (\Xi(s))^2 \right)$$

Furtula et al. (2010) acquainted with a new topological index named “augmented Zagreb index” and is characterized as:

$$AZI(G) = \sum_{rs \in E(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r) + \Xi(s) - 2} \right)^3$$

Balaban (1982) and Balaban and Quintas (1983) announced a new topological index for a graph G of order p , size q as:

$$J(G) = \frac{q}{q-p+2} \sum_{rs \in E(G)} \frac{1}{\sqrt{\Xi(r)\Xi(s)}}$$

For more details about these indices see: Akhter et al. (2016), Ali et al. (2019), Liu et al. (2020a, 2020b), Raza (2020a, 2020b), Raza and Ali (2020), and Raza and Sukaiti (2020).

3 General entropy of graph

In 2014, Chen et al. (2014) familiarized the definition of the entropy of edge partisan graph. The entropy of edge partisan graph is characterized in Eq. 1:

$$ENT_{\psi}(G) = \sum_{r's' \in E(G)} \frac{\psi(r's')}{\sum_{rs \in E(G)} \psi(rs)} \log \left[\frac{\psi(r's')}{\sum_{rs \in E(G)} \psi(rs)} \right] \quad (1)$$

3.1 The first Zagreb entropy

If $\psi(rs) = \Xi(r) + \Xi(s)$, then:

$$\sum_{rs \in E(G)} \psi(rs) = \sum_{rs \in E(G)} (\Xi(r) + \Xi(s)) = M_1(G)$$

Now Eq. 1 is converted and called the first Zagreb entropy:

$$ENT_{M_1}(G) = \log(M_1(G)) - \frac{1}{M_1(G)} \log \left[\prod_{rs \in E_1(G)} [\Xi(r) + \Xi(s)]^{[\Xi(r) + \Xi(s)]} \right] \quad (2)$$

3.2 The second Zagreb entropy

If $\psi(rs) = \Xi(r) \times \Xi(s)$, then:

$$\sum_{rs \in E(G)} \psi(rs) = \sum_{rs \in E(G)} (\Xi(r) \times \Xi(s)) = M_2(G)$$

Now Eq. 1 is converted and called the second Zagreb entropy:

$$ENT_{M_2}(G) = \log(M_2(G)) - \frac{1}{M_2(G)} \log \left[\prod_{rs \in E(G)} [\Xi(r) \times \Xi(s)]^{[\Xi(r) \times \Xi(s)]} \right] \quad (3)$$

3.3 The hyper Zagreb entropy

If $\psi(rs) = [\Xi(r) + \Xi(s)]^2$, then:

$$\sum_{rs \in E(G)} \psi(rs) = \sum_{rs \in E(G)} [\Xi(r) + \Xi(s)]^2 = HM(G)$$

Now Eq. 1 is converted and called the hyper Zagreb entropy:

$$ENT_{HM}(G) = \log(HM(G)) - \frac{1}{HM(G)} \log \left[\prod_{rs \in E(G)} [\Xi(r) + \Xi(s)]^2 \right] \quad (4)$$

3.4 The forgotten entropy

If $\psi(rs) = [\Xi(r)^2 + \Xi(s)^2]$, then:

$$\sum_{rs \in E(G)} \psi(rs) = \sum_{rs \in E(G)} [\Xi(r)^2 + \Xi(s)^2] = F(G)$$

Now Eq. 1 is converted and called the forgotten entropy:

$$ENT_F(G) = \log(F(G)) - \frac{1}{F(G)} \log \left[\prod_{rs \in E(G)} [\Xi(r)^2 + \Xi(s)^2] \right] \quad (5)$$

3.5 The augmented Zagreb entropy

If $\psi(rs) = \left(\frac{\Xi(r)\Xi(s)}{\Xi(r) + \Xi(s) - 2} \right)^3$, then:

$$\sum_{rs \in E(G)} \psi(rs) = \sum_{rs \in E(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r) + \Xi(s) - 2} \right)^3 = AZI(G)$$

Now Eq. 1 is converted and called the augmented Zagreb entropy:

$$ENT_{AZI}(G) = \log(AZI(G)) - \frac{1}{AZI(G)} \log \left[\prod_{rs \in E(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r) + \Xi(s) - 2} \right)^3 \right] \quad (6)$$

3.6 The Balaban entropy

If $\psi(rs) = \frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}}$, then:

$$\sum_{rs \in E(G)} \psi(rs) = \frac{q}{q-p+2} \sum_{rs \in E(G)} \frac{1}{\sqrt{\Xi(r)\Xi(s)}} = J(G)$$

Now Eq. 1 is converted and called the Balaban entropy:

$$ENT_J(G) = \log(J(G)) - \frac{1}{J(G)} \log \left[\prod_{rs \in E(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right] \right] \quad (7)$$

4 Crystallographic structure of first carbon nanosheet $T^1C_4C_8(S)[m, n]$

A $C_4C_8(S)$ nanosheet is a trivalent ornamentation prepared by blinking tetragons C_4 and octagons C_8 . There are two categories of nanosheets which canister be completed by C_4 and C_8 following the trivalent ornamentation which we mention to as $T^1C_4C_8(S)[m, n]$ and $T^2C_4C_8(R)[m, n]$. $T^1C_4C_8(S)[m, n]$ nanosheet is the two-dimensional lattice of $TUC_4C_8(S)[m, n]$, where m and n are significant restrictions in Figure 1. In this segment, we deliberate the first kind of nanosheet i.e. $T^1C_4C_8(S)[m, n]$ in which C_4 acts as a tetragonal and m and n are the quantity of octagons in any pillar and racket individually. Figure 2 portrays the Type-I $C_4C_8(S)$ nanosheet $T^1C_4C_8(S)[m, n]$. The vertex and edge cardinalities of this organic graph are $8mn$ and $12mn - 2(m + n)$ correspondingly.

The vertex barrier of $T^1C_4C_8(S)[m, n]$ established on degrees of respectively vertex is portrayed in Table 1. Also the edge barrier of $T^1C_4C_8(S)[m, n]$ centered on degrees of end vertices of apiece edge are depicted in Table 2.

Figure 1: A $TUC_4C_8(S)[m, n]$ nanotube.

Figure 2: Type-I $C_4C_8(S)$ nanosheet $T^1C_4C_8(S)[m, n]$.Table 1: Vertex partition of $T^1C_4C_8(S)[m, n]$.

$\Xi(r)$	Frequency	Set of vertices
2	$4m + 4n$	V_1
3	$8mn - 4m - 4n$	V_2

Table 2: Edge partition of $T^1C_4C_8(S)[m, n]$.

$(\Xi(r), \Xi(s))$	Frequency	Set of edges
(2, 2)	$2m + 2n + 4$	E_1
(3, 2)	$4m + 4n - 8$	E_2
(3, 3)	$12mn - 8m - 8n + 4$	E_3

4.1 Results for carbon nanosheet $T^1C_4C_8(S)[m, n]$

4.1.1 The first Zagreb entropy of $T^1C_4C_8(S)[m, n]$

Now using Eq. 2 and Table 2, we computed following results. The first Zagreb index by using Table 2 is:

$$M_1(G) = 72mn - 20(m + n)$$

Now Eq. 2 (with Table 2) can take the following form:

$$\begin{aligned} ENT_{M_1}(T^1C_4C_8(S)) &= \log(M_1(G)) - \frac{1}{M_1(G)} \log \left[\prod_{rs \in E_1(G)} [\Xi(r) + \Xi(s)]^{\Xi(r) + \Xi(s)} \times \prod_{rs \in E_2(G)} [\Xi(r) + \Xi(s)]^{\Xi(r) + \Xi(s)} \times \prod_{rs \in E_3(G)} [\Xi(r) + \Xi(s)]^{\Xi(r) + \Xi(s)} \right] \\ &= \log(M_1) - \frac{1}{(M_1)} \log \left[\left[(2m + 2n + 4) \times (256) \right] \times \left[(4m + 4n - 8) \times (3125) \right] \times \left[(12mn - 8m - 8n + 4) \times (46656) \right] \right] \\ &= \log(72mn - 20(m + n)) - \frac{\log[(2m + 2n + 4) \times (256)]}{(72mn - 20(m + n))} - \frac{\log[(4m + 4n - 8) \times (3125)]}{(72mn - 20(m + n))} - \frac{\log[(12mn - 8m - 8n + 4) \times (46656)]}{(72mn - 20(m + n))} \end{aligned}$$

4.1.2 The second Zagreb entropy of $T^1C_4C_8(S)[m, n]$

$$M_2(G) = 108mn - 40(m + n) + 4$$

Now using Eq. 3 and Table 2, we computed following results. The second Zagreb index by using Table 2 is:

Now Eq. 3 (with Table 2) can take the following form:

$$\begin{aligned} ENT_{M_2}(T^1C_4C_8(S)) &= \log(M_2(G)) - \frac{1}{M_2(G)} \log \left[\prod_{rs \in E_1(G)} [\Xi(r) \times \Xi(s)]^{\Xi(r) \times \Xi(s)} \times \prod_{rs \in E_2(G)} [\Xi(r) \times \Xi(s)]^{\Xi(r) \times \Xi(s)} \times \prod_{rs \in E_3(G)} [\Xi(r) \times \Xi(s)]^{\Xi(r) \times \Xi(s)} \right] \\ &= \log(M_2) - \frac{1}{(M_2)} \log \left[\left[(2m + 2n + 4) \times (256) \right] \times \left[(4m + 4n - 8) \times (46656) \right] \times \left[(12mn - 8m - 8n + 4) \times (9^9) \right] \right] \\ &= \log(108mn - 40(m + n) + 4) - \frac{\log[(2m + 2n + 4) \times (256)]}{(108mn - 40(m + n) + 4)} - \frac{\log[(4m + 4n - 8) \times (46656)]}{(108mn - 40(m + n) + 4)} - \frac{\log[(12mn - 8m - 8n + 4) \times (9^9)]}{(108mn - 40(m + n) + 4)} \end{aligned}$$

4.1.3 The hyper Zagreb entropy of $T^1C_4C_8(S)[m, n]$

$$HM(G) = 432mn - 156(m+n) + 8$$

Now using Eq. 4 and Table 2, we computed following result. By using Table 2, we have:

Now Eq. 4 (with Table 2) is reduced to the following form:

$$\begin{aligned} ENT_{HM}(T^1C_4C_8(S)) &= \log(HM(G)) - \frac{1}{HM(G)} \log \left[\prod_{rs \in E_1(G)} \left[(\Xi(r) + \Xi(s))^2 \right]^{\left[(\Xi(r) + \Xi(s))^2 \right]} \times \prod_{rs \in E_2(G)} \left[(\Xi(r) + \Xi(s))^2 \right]^{\left[(\Xi(r) + \Xi(s))^2 \right]} \times \prod_{rs \in E_3(G)} \left[(\Xi(r) + \Xi(s))^2 \right]^{\left[(\Xi(r) + \Xi(s))^2 \right]} \right] \\ &= \log(HM(G)) - \frac{1}{HM(G)} \log \left[\left[(2m+2n+4) \times (16)^{(16)} \right] \times \left[(4m+4n-8) \times (25)^{(25)} \right] \times \left[(12mn-8m-8n+4) \times (36)^{(36)} \right] \right] \\ &= \log(432mn - 156(m+n) + 8) - \frac{\log \left[(2m+2n+4) \times (16)^{(16)} \right]}{(432mn - 156(m+n) + 8)} - \frac{\log \left[(4m+4n-8) \times (25)^{(25)} \right]}{(432mn - 156(m+n) + 8)} - \frac{\log \left[(12mn-8m-8n+4) \times (36)^{(36)} \right]}{(432mn - 156(m+n) + 8)} \end{aligned}$$

4.1.4 The forgotten Zagreb entropy of $T^1C_4C_8(S)[m, n]$

$$F(G) = 216mn - 76(m+n)$$

Now using Eq. 5 and Table 2, we got following expressions. By using Table 2, we have:

Now Eq. 4 (with Table 2) is reduced to the following form:

$$\begin{aligned} ENT_F(T^1C_4C_8(S)) &= \log(F(G)) - \frac{1}{F(G)} \log \left[\prod_{rs \in E_1(G)} \left[(\Xi(r))^2 + (\Xi(s))^2 \right]^{\left[(\Xi(r))^2 + (\Xi(s))^2 \right]} \times \prod_{rs \in E_2(G)} \left[(\Xi(r))^2 + (\Xi(s))^2 \right]^{\left[(\Xi(r))^2 + (\Xi(s))^2 \right]} \times \prod_{rs \in E_3(G)} \left[(\Xi(r))^2 + (\Xi(s))^2 \right]^{\left[(\Xi(r))^2 + (\Xi(s))^2 \right]} \right] \\ &= \log(F(G)) - \frac{1}{F(G)} \log \left[\left[(2m+2n+4) \times (8)^{(8)} \right] \times \left[(4m+4n-8) \times (13)^{(13)} \right] \times \left[(12mn-8m-8n+4) \times (18)^{(18)} \right] \right] \\ &= \log(216mn - 76(m+n)) - \frac{\log \left[(2m+2n+4) \times (16)^{(16)} \right]}{(216mn - 76(m+n))} - \frac{\log \left[(4m+4n-8) \times (25)^{(25)} \right]}{(216mn - 76(m+n))} - \frac{\log \left[(12mn-8m-8n+4) \times (36)^{(36)} \right]}{(216mn - 76(m+n))} \end{aligned}$$

4.1.5 The augmented Zagreb entropy of $T^1C_4C_8(S)[m, n]$

$$AZI(G) = \frac{2187}{16}mn - \frac{345}{5}(m+n) + \frac{217}{16}$$

Now using Eq. 5 and Table 2, we got following expressions. By using Table 2, we have:

Now Eq. 6 (with Table 2) becomes:

$$\begin{aligned}
\text{ENT}_{\text{AZI}}(T^1C_4C_8(S)) &= \log(\text{AZI}(G)) \\
&- \frac{1}{\text{AZI}(G)} \log \left[\prod_{rs \in E_1(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^{3 \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)} \times \prod_{rs \in E_2(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^{3 \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)} \times \prod_{rs \in E_3(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^{3 \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)} \right] \\
&= \log(\text{AZI}(G)) - \frac{1}{(\text{AZI}(G))} \log \left[\left[(2m+2n+4) \times (8)^{(8)} \right] \times \left[(4m+4n-8) \times (8)^{(8)} \right] \times \left[(12mn-8m-8n+4) \times \left(\frac{9^3}{4^3} \right)^{\left(\frac{9^3}{4^3} \right)} \right] \right] \\
&= \log \left(\frac{2187}{16} mn - \frac{345}{5} (m+n) + \frac{217}{16} \right) \\
&\quad - \frac{\log \left[(2m+2n+4) \times (8)^{(8)} \right]}{\left(\frac{2187}{16} mn - \frac{345}{5} (m+n) + \frac{217}{16} \right)} - \frac{\log \left[(4m+4n-8) \times (8)^{(8)} \right]}{\left(\frac{2187}{16} mn - \frac{345}{5} (m+n) + \frac{217}{16} \right)} - \frac{\log \left[(12mn-8m-8n+4) \times \left(\frac{9^3}{4^3} \right)^{\left(\frac{9^3}{4^3} \right)} \right]}{\left(\frac{2187}{16} mn - \frac{345}{5} (m+n) + \frac{217}{16} \right)}
\end{aligned}$$

4.1.6 The Balaban entropy of $T^1C_4C_8(S)[m, n]$

$$J(G) = \frac{12mn-2m-2n}{4mn-2m-2n+2} \left(4mn + \left(\frac{4}{\sqrt{6}} - \frac{5}{3} \right) (m+n) + \frac{10}{3} - \frac{8}{\sqrt{6}} \right)$$

Now using Eq. 7 and Table 2, we move in the following way. By using Table 2, we have:

Equation 7 (with Table 2) takes the following form:

$$\begin{aligned}
\text{ENT}_J(T^1C_4C_8(S)) &= \log(J(G)) \\
&- \frac{1}{J(G)} \log \left[\prod_{rs \in E_1(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]^{\left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]} \times \prod_{rs \in E_2(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]^{\left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]} \times \prod_{rs \in E_3(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]^{\left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]} \right] \\
&= \log(J(G)) - \frac{1}{(J(G))} \log \left[\left[(2m+2n+4) \times \left[\frac{q}{2(q-p+2)} \right]^{\left[\frac{q}{2(q-p+2)} \right]} \right] \times \left[(4m+4n-8) \times \left[\frac{q}{\sqrt{6}(q-p+2)} \right]^{\left[\frac{q}{\sqrt{6}(q-p+2)} \right]} \right] \times \left[(12mn-8m-8n+4) \times \left[\frac{q}{3(q-p+2)} \right]^{\left[\frac{q}{3(q-p+2)} \right]} \right] \right]
\end{aligned}$$

$$\begin{aligned}
& \log \left[(2m+2n+4) \times \left[\frac{q}{2(q-p+2)} \right]^{\left[\frac{q}{2(q-p+2)} \right]} \right] \\
& = \log(J(G)) - \frac{\log \left[(2m+2n+4) \times \left[\frac{q}{2(q-p+2)} \right]^{\left[\frac{q}{2(q-p+2)} \right]} \right]}{(J(G))} \\
& \log \left[(4m+4n-8) \times \left[\frac{q}{\sqrt{6}(q-p+2)} \right]^{\left[\frac{q}{\sqrt{6}(q-p+2)} \right]} \right] \quad \log \left[(12mn-8m-8n+4) \times \left[\frac{q}{3(q-p+2)} \right]^{\left[\frac{q}{3(q-p+2)} \right]} \right] \\
& \frac{\log \left[(4m+4n-8) \times \left[\frac{q}{\sqrt{6}(q-p+2)} \right]^{\left[\frac{q}{\sqrt{6}(q-p+2)} \right]} \right]}{(J(G))} \quad \frac{\log \left[(12mn-8m-8n+4) \times \left[\frac{q}{3(q-p+2)} \right]^{\left[\frac{q}{3(q-p+2)} \right]} \right]}{(J(G))}
\end{aligned}$$

5 Carbon nanosheet $T^2C_4C_8(R)[m, n]$

A $C_4C_8(R)$ nanosheet is a trivalent decoration prepared by ashing rhombus C_4 and octagons C_8 . We talk about this nanosheet as $T^2C_4C_8(R)[m, n]$. This nanosheet is the two-dimensional lattice of $TUC_4C_8(R)[m, n]$, where m and n are essential limitations in Figure 3. In this section we discourse $T^2C_4C_8(R)[m, n]$ in which C_4 entertainments as a rhombus and m and n are quantity of octagons in any pillar and row correspondingly. Figure 4 depicts the type-II $C_4C_8(R)$ nanosheet $T^2C_4C_8(R)[m, n]$. The vertex and edge cardinalities of this organic graph are $4mn + 4(m + n) + 4$ and $6mn + 5(m + n) + 4$ correspondingly.

The vertex barrier of $T^2C_4C_8(R)[m, n]$ grounded on degrees of each vertex is portrayed in Table 3. Also the edge dividing wall of $T^2C_4C_8(R)[m, n]$ centered on degrees of expiration vertices of respectively edge are showed in Table 4.

Figure 3: A $TUC_4C_8(R)[m, n]$ nanotube.

Figure 4: Type-II $C_4C_8(R)$ nanosheet $T^2C_4C_8(R)[m, n]$.

5.1 Results for carbon nanosheet $T^2C_4C_8(R)[m, n]$

5.1.1 The first Zagreb entropy of $T^2C_4C_8(R)[m, n]$

Now using Eq. 2 and Table 4, we have:

$$M_1(G) = 36mn + 26(m + n) + 16$$

Equation 2 (with Table 4) is converted into the following form:

$$ENT_{M_1}(T^2C_4C_8(R)) = \log(M_1) - \frac{1}{(M_1)} \log \left[\prod_{rs \in E_1(G)} [\Xi(r) + \Xi(s)]^{\left[\frac{\Xi(r) + \Xi(s)}{2} \right]} + \prod_{rs \in E_2(G)} [\Xi(r) + \Xi(s)]^{\left[\frac{\Xi(r) + \Xi(s)}{2} \right]} + \prod_{rs \in E_3(G)} [\Xi(r) + \Xi(s)]^{\left[\frac{\Xi(r) + \Xi(s)}{2} \right]} \right]$$

Table 3: Vertex partition of $T^2C_4C_8(R)[m, n]$.

$\Xi(r)$	Frequency	Set of vertices
2	$2m + 2n + 4$	V_1
3	$4mn + 2m + 2n$	V_2

Table 4: Edge partition of $T^2C_4C_8(R)[m, n]$.

$(\Xi(r), \Xi(r))$	Frequency	Set of edges
(2, 2)	4	E_1
(3, 2)	$4m + 4n$	E_2
(3, 3)	$6mn + m + n$	E_3

$$\begin{aligned}
&= \log(M_1) - \frac{1}{(M_1)} \log \left[\left[(4) \times (256) \right] \times \left[(4m + 4n) \times (3125) \right] \times \left[(6mn + m + n) \times (46656) \right] \right] \\
&= \log(36mn + 26(m + n) + 16) - \frac{\log \left[(4) \times (256) \right]}{(36mn + 26(m + n) + 16)} - \frac{\log \left[(4m + 4n) \times (3125) \right]}{(36mn + 26(m + n) + 16)} - \frac{\log \left[(6mn + m + n) \times (46656) \right]}{(36mn + 26(m + n) + 16)}
\end{aligned}$$

5.1.2 The second Zagreb entropy of $T^2C_4C_8(S)[m, n]$

Now using Eq. 3 and Table 4, we computed the first Zagreb entropy in the following way:

By using Table 4, we have:

$$M_2(G) = 54mn + 33(m + n) + 16$$

Equation 3 (with Table 4) becomes:

$$\begin{aligned}
\text{ENT}_{M_2}(T^2C_4C_8(R)) &= \log(M_2) - \frac{1}{(M_2)} \log \left[\prod_{rs \in E_1(G)} [\Xi(r) \times \Xi(s)]^{\left[\Xi(r) \times \Xi(s) \right]} + \prod_{rs \in E_2(G)} [\Xi(r) \times \Xi(s)]^{\left[\Xi(r) \times \Xi(s) \right]} + \prod_{rs \in E_3(G)} [\Xi(r) \times \Xi(s)]^{\left[\Xi(r) \times \Xi(s) \right]} \right] \\
&= \log(M_2) - \frac{1}{(M_2)} \log \left[\left[(4) \times (256) \right] \times \left[(4m + 4n) \times (46656) \right] \times \left[(6mn + m + n) \times (387420489) \right] \right] \\
&= \log(54mn + 33(m + n) + 16) - \frac{\log \left[(4) \times (256) \right]}{(54mn + 33(m + n) + 16)} - \frac{\log \left[(4m + 4n) \times (46656) \right]}{(54mn + 33(m + n) + 16)} - \frac{\log \left[(6mn + m + n) \times (387420489) \right]}{(54mn + 33(m + n) + 16)}
\end{aligned}$$

5.1.3 The hyper Zagreb entropy of $T^2C_4C_8(R)[m, n]$

$$HM(G) = 216mn + 136(m + n) + 64$$

Now using Eq. 4 and Table 4, we computed the following result:

$$\begin{aligned}
\text{ENT}_{HM}(T^2C_4C_8(R)) &= \log(HM) - \frac{1}{(HM)} \log \left[\prod_{rs \in E_1(G)} \left[(\Xi(r) + \Xi(s))^2 \right]^{\left[(\Xi(r) + \Xi(s))^2 \right]} + \prod_{rs \in E_2(G)} \left[(\Xi(r) + \Xi(s))^2 \right]^{\left[(\Xi(r) + \Xi(s))^2 \right]} + \prod_{rs \in E_3(G)} \left[(\Xi(r) + \Xi(s))^2 \right]^{\left[(\Xi(r) + \Xi(s))^2 \right]} \right] \\
&= \log(HM) - \frac{1}{(HM)} \log \left[\left[(4) \times (16)^{(16)} \right] \times \left[(4m + 4n) \times (25)^{(25)} \right] \times \left[(6mn + m + n) \times (36)^{(36)} \right] \right]
\end{aligned}$$

$$= \log \left(216mn + 136(m+n) + 64 \right) - \frac{\log \left[(4) \times (16)^{(16)} \right]}{\left(216mn + 136(m+n) + 64 \right)} - \frac{\log \left[(4m+4n) \times (25)^{(25)} \right]}{\left(216mn + 136(m+n) + 64 \right)} - \frac{\log \left[(6mn+m+n) \times (36)^{(36)} \right]}{\left(216mn + 136(m+n) + 64 \right)}$$

5.1.4 The forgotten Zagreb entropy of $T^2C_4C_8(R)[m, n]$

$$F(G) = 108mn + 70(m+n) + 32$$

Using Table 4, we obtained:

Equation 5 (with Table 4) becomes:

$$\begin{aligned} \text{ENT}_F(T^2C_4C_8(R)) &= \log(F(G)) \\ &- \frac{1}{F(G)} \log \left[\prod_{rs \in E_1(G)} \left[(\Xi(r))^2 + (\Xi(s))^2 \right]^{\left[(\Xi(r))^2 + (\Xi(s))^2 \right]} \times \prod_{rs \in E_2(G)} \left[(\Xi(r))^2 + (\Xi(s))^2 \right]^{\left[(\Xi(r))^2 + (\Xi(s))^2 \right]} \times \prod_{rs \in E_3(G)} \left[(\Xi(r))^2 + (\Xi(s))^2 \right]^{\left[(\Xi(r))^2 + (\Xi(s))^2 \right]} \right] \\ &= \log(F(G)) - \frac{1}{F(G)} \log \left[\left[(4) \times (8)^{(8)} \right] \times \left[(4m+4n) \times (13)^{(13)} \right] \times \left[(6mn+m+n) \times (18)^{(18)} \right] \right] \\ &= \log \left(108mn + 70(m+n) + 32 \right) - \frac{\log \left[(2m+2n+4) \times (16)^{(16)} \right]}{\left(108mn + 70(m+n) + 32 \right)} - \frac{\log \left[(4m+4n-8) \times (25)^{(25)} \right]}{\left(108mn + 70(m+n) + 32 \right)} - \frac{\log \left[(12mn-8m-8n+4) \times (36)^{(36)} \right]}{\left(108mn + 70(m+n) + 32 \right)} \end{aligned}$$

5.1.5 The augmented Zagreb entropy of $T^2C_4C_8(S)[m, n]$

$$\text{AZI}(G) = \frac{2187}{32}mn - \frac{2777}{64}(m+n) + 32$$

Using Table 2, we have:

$$\begin{aligned} \text{ENT}_{\text{AZI}}(T^2C_4C_8(R)) &= \log(\text{AZI}(G)) \\ &- \frac{1}{\text{AZI}(G)} \log \left[\prod_{rs \in E_1(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^3 \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^{\left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)} \times \prod_{rs \in E_2(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^3 \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^{\left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)} \times \prod_{rs \in E_3(G)} \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^3 \left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)^{\left(\frac{\Xi(r)\Xi(s)}{\Xi(r)+\Xi(s)-2} \right)} \right] \\ &= \log(\text{AZI}(G)) - \frac{1}{\text{AZI}(G)} \log \left[\left[(4) \times (8)^{(8)} \right] \times \left[(4m+4n) \times (8)^{(8)} \right] \times \left[(6mn+m+n) \times \left(\frac{729}{64} \right)^{\left(\frac{729}{64} \right)} \right] \right] \\ &= \log \left(\frac{2187}{32}mn - \frac{2777}{64}(m+n) + 32 \right) \\ &- \frac{\log \left[(4) \times (8)^{(8)} \right]}{\left(\frac{2187}{32}mn - \frac{2777}{64}(m+n) + 32 \right)} - \frac{\log \left[(4m+4n) \times (8)^{(8)} \right]}{\left(\frac{2187}{32}mn - \frac{2777}{64}(m+n) + 32 \right)} - \frac{\log \left[(6mn+m+n) \times \left(\frac{729}{64} \right)^{\left(\frac{729}{64} \right)} \right]}{\left(\frac{2187}{32}mn - \frac{2777}{64}(m+n) + 32 \right)} \end{aligned}$$

5.1.6 The Balaban entropy of $T^2C_4C_8(R)[m, n]$

By using Table 4, we obtained:

$$J(G) = \frac{6mn + 5(m+n) + 4}{2mn + (m+n) + 2} \left[2mn + \left(\frac{1}{3} + \frac{4}{\sqrt{6}} \right) (m+n) + 2 \right]$$

Equation 7 (with Table 4) takes the following form:

$$\begin{aligned} ENT_J(T^2C_4C_8(R)) &= \log(J(G)) - \frac{1}{J(G)} \log \left[\prod_{r \in E_1(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]^{\left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]} \times \prod_{r \in E_2(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]^{\left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]} \times \prod_{r \in E_3(G)} \left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]^{\left[\frac{q}{q-p+2} \times \frac{1}{\sqrt{\Xi(r)\Xi(s)}} \right]} \right] \\ &= \log(J(G)) - \frac{1}{J(G)} \log \left[\left(4 \times \left[\frac{q}{2(q-p+2)} \right]^{\left[\frac{q}{2(q-p+2)} \right]} \right) \times \left((4m+4n) \times \left[\frac{q}{\sqrt{6}(q-p+2)} \right]^{\left[\frac{q}{\sqrt{6}(q-p+2)} \right]} \right) \times \left((6mn+m+n) \times \left[\frac{q}{3(q-p+2)} \right]^{\left[\frac{q}{3(q-p+2)} \right]} \right) \right] \\ &= \log(J(G)) - \frac{\log \left(4 \times \left[\frac{q}{2(q-p+2)} \right]^{\left[\frac{q}{2(q-p+2)} \right]} \right)}{J(G)} - \frac{\log \left((4m+4n) \times \left[\frac{q}{\sqrt{6}(q-p+2)} \right]^{\left[\frac{q}{\sqrt{6}(q-p+2)} \right]} \right)}{J(G)} - \frac{\log \left((6mn+m+n) \times \left[\frac{q}{3(q-p+2)} \right]^{\left[\frac{q}{3(q-p+2)} \right]} \right)}{J(G)} \end{aligned}$$

6 Comparisons and discussion for $T^1C_4C_8(S)[m, n]$

Since the degree based entropy has part of utilization in various parts of science, in particular pharmaceutical,

science, organic medications and software engineering. So the numerical and graphical portrayal of these determined outcomes are useful to researcher. So in this area, we have registered numerically all degree based entropies for various estimations of m, n for $T^1C_4C_8(S)[m, n]$. Furthermore, we develop Tables 5 and 6

Table 5: Comparison of first Zagreb entropy and second Zagreb entropy for $T^1C_4C_8(S)[m, n]$.

$[m, n]$	ENT_{M_1}	ENT_{M_2}
[2, 2]	2.25	2.37
[3, 3]	2.69	2.84
[4, 4]	2.98	3.14
[5, 5]	3.19	3.35
[6, 6]	3.36	3.53
[7, 7]	3.51	3.67
[8, 8]	3.63	3.79
[9, 9]	3.74	3.90
[10, 10]	3.83	4.01

Table 6: Comparison of ENT_{HM} , ENT_F , ENT_{AZI} , and ENT_J entropies for $T^1C_4C_8(S)[m, n]$.

$[m, n]$	ENT_{HM}	ENT_F	ENT_{AZI}	ENT_J
[2, 2]	2.94	2.66	2.51	1.74
[3, 3]	3.43	3.14	2.96	2.08
[4, 4]	3.73	3.44	3.25	2.33
[5, 5]	3.95	3.36	3.47	2.51
[6, 6]	4.13	3.83	3.64	2.67
[7, 7]	4.27	3.97	3.78	2.80
[8, 8]	4.40	4.10	3.90	2.91
[9, 9]	4.50	4.20	4.01	3.01
[10, 10]	4.60	4.30	4.11	3.10

for little estimations of m , n for degree based entropy to numerical correlation for the structure of $T^1C_4C_8$ (S) $[m, n]$. Presently, from Tables 5 and 6, we can without much of a stretch see that all the estimations of entropy are in expanding request as the estimations of m ; n are increments. The graphical portrayals of registered outcomes are delineated in Figures 5-7 for specific estimations of m , n .

7 Comparisons and discussion for $T^2C_4C_8(R)[m, n]$

Since the degree based entropy has parcel of utilization in various parts of science, in particular pharmaceutical, science, natural medications and software engineering. So the numerical and graphical portrayal of these determined outcomes are useful to researcher.

Figure 5: (a) The first Zagreb entropy, (b) the second Zagreb entropy.

Figure 6: (a) The hyper Zagreb entropy, (b) the forgotten entropy.

Figure 7: (a) The augmented Zagreb entropy, (b) the Balaban entropy.

So in this area, we have figured numerically all degree based entropies for various estimations of m ; n for $T^2C_4C_8(R)[m, n]$. Moreover, we build Tables 7 and 8 for little estimations of m , n for degree based entropy to numerical correlation for the structure of $T^2C_4C_8(R)[m, n]$. Presently, from Tables 7 and 8, we can without much of a stretch see that all the estimations of entropy are in expanding

request as the estimations of m ; n are increments. The graphical portrayals of processed outcomes are delineated in Figures 8-10 for specific estimations of m , n .

Funding: The research was supported by the National Natural Science Foundation of China (Grant Nos. 11971142, 11871202, 61673169, 11701176, 11626101, 11601485).

Table 7: Comparison of first Zagreb entropy and second Zagreb entropy for $T^2C_4C_8(S)[m, n]$.

$[m, n]$	ENT_{M_1}	ENT_{M_2}
[2, 2]	2.37	2.51
[3, 3]	2.67	2.82
[4, 4]	2.88	3.04
[5, 5]	3.06	3.22
[6, 6]	3.20	3.36
[7, 7]	3.32	3.49
[8, 8]	3.43	3.60
[9, 9]	3.53	3.69
[10, 10]	3.61	4.78

Table 8: Comparison of ENT_{HM} , ENT_F , ENT_{AZI} , and ENT_J entropies for $T^2C_4C_8(S)[m, n]$.

$[m, n]$	ENT_{HM}	ENT_F	ENT_{AZI}	ENT_J
[2, 2]	3.09	2.81	2.62	1.72
[3, 3]	3.41	3.12	2.92	1.99
[4, 4]	3.64	3.34	3.15	2.19
[5, 5]	3.82	3.52	3.32	2.35
[6, 6]	3.96	3.67	3.47	2.49
[7, 7]	4.09	3.79	3.59	2.60
[8, 8]	4.20	3.90	3.70	2.70
[9, 9]	4.30	3.99	3.80	2.79
[10, 10]	4.38	4.08	3.88	2.88

Figure 8: (a) The first Zagreb entropy, (b) the second Zagreb entropy.

Figure 9: (a) The hyper Zagreb entropy, (b) the forgotten entropy.

Figure 10: (a) The augmented Zagreb entropy, (b) the Balaban entropy.

References

- Akhter S., Imran M., Raza Z., On the general sum-connectivity index and general Randic index of cacti. *J. Ineq. Applic.*, 2016, 1, 300-310.
- Ali A., Raza Z., Bhatti A.A., Some vertex-degree-based topological indices of cacti. *Ars Combinatoria*, 2019, 144, 195-206.
- Assaye B., Alamneh M., Mishra L.N., Mebrat Y., Dual skew Heyting almost distributive lattices. *Appl. Math. Nonli. Sci.*, 2019, 4(1), 151-162.
- Balaban A.T., Highly discriminating distance-based topological index. *Chem. Phys. Lett.*, 1982, 89(5), 399-404.
- Balaban A.T., Quintas L.V., The smallest graphs, trees, and 4-trees with degenerate topological index. *J. Math. Chem.*, 1983, 14, 213-233.
- Basavanagoud B., Gao W., Patil S., Desai V.R., Mirajkar K.G., Pooja B., Computing First Zagreb index and F-index of New C-products of Graphs. *Appl. Math. Nonlinear Sci.*, 2017, 2(1), 285-298.
- Bonchev D., Complexity in Chemistry, Introduction and Fundamentals. Taylor and Francis, Boca Raton, FL, USA, 2003, 7, 157-185.
- Chen Z., Dehmer M., Shi Y., A note on distance-based graph entropies. *Entropy*, 2014, 16(10), 5416-5427.
- Dehmer M., Information processing in complex networks: Graph entropy and information functionals. *Appl. Math. Comput.*, 2008, 201(1-2), 82-94.
- Dehmer M., Grabner M., The discrimination power of molecular identification numbers revisited. *Match Commun. Math. Comput. Chem.*, 2013, 69(3), 785-794.
- Dehmer M., Mowshowitz A., A history of graph entropy measures. *Info. Sci.*, 2011, 181(1), 57-78.
- Dehmer M., Sivakumar L., Varmuza K., Uniquely discriminating molecular structures using novel eigen-value-based descriptors. *Match. Commun. Math. Comput. Chem.*, 2012, 67(1), 147.
- Furtula B., Graovac A., Vukicevic D., Augmented Zagreb index. *J. Math. Chem.*, 2010, 48(2), 370-380.
- Furtula B., Gutman I., A forgotten topological index. *J. Math. Chem.*, 2015, 53(4), 1184-1190.
- Gao W., Farahani M.R., Degree-based indices computation for special chemical molecular structures using edge dividing method. *Appl. Math. Nonlinear Sci.*, 2016, 1(1), 99-122.
- Gao W., Siddiqui M.K., Naeem M., Rehman N.A., Topological characterization of carbon graphite and crystal cubic carbon structures. *Molecules*, 2017, 22(9), 1496.
- Gao W., Wu H., Siddiqui M.K., Baig A. Q., Study of biological networks using graph theory. *Saudi J. Biol. Sci.*, 2018, 25(6), 1212-1219.
- Gutman I., Das K.C., The first Zagreb index 30 years after. *Match Commun. Math. Comput. Chem.*, 2004, 50(1), 83-92.
- Gutman I., Trinajstić N., Graph theory and molecular orbitals. Total ρ – electron energy of alternant hydrocarbons. *Chem. Phys. Lett.*, 1972, 17(4), 535-538.
- Hosamani S.M., Kulkarni B.B., Boli R.G., Gadag V.M., QSPR analysis of certain graph theoretical matrices and their corresponding energy. *Appl. Math. Nonli. Sci.*, 2017, 2(1), 131-150.
- Imran M., Siddiqui M.K., Naeem M., Iqbal M.A., On topological properties of symmetric chemical structures. *Symmetry*, 2018, 10(5), 173-183.
- Liu J.B., Baig A.Q., Imran M., Khalid W., Saeed M., Farahani M.R., Computation of bond incident degree (BID) indices of complex structures in drugs. *Eurasian Chem. Commun.*, 2020a, 2(6), 672-679.
- Liu J.B., Raza Z., Javaid M., Zagreb Connection Numbers for Cellular Neural Networks. *Disc. Dynamics Nat. Society*, 2020b, 1-15.
- Morowitz H.J., Some order-disorder considerations in living systems. *Bull. Math. Biophys.*, 1955, 17(2), 81-86.
- Quastler H., Information theory in biology. *Bull. Math. Biol.*, 1954, 8, 183-185.
- Rashevsky N., Life, information theory and topology. *Bull. Math. Biophys.*, 1955, 17(3), 229-235.
- Raza Z., The expected values of arithmetic bond connectivity and geometric indices in random phenylene chains. *Heliyon*, 2020a, 6(7), 55-69.
- Raza Z., The harmonic and second Zagreb indices in random polyphenyl and spiro chains. *Polycyclic Aromatic Compounds*, 2020b, 1-10.
- Raza Z., Ali A., Bounds on the Zagreb indices for molecular (n, m) -graphs. *Int. J. Quantum Chem.*, 2020, 120(18), 45-55.
- Raza Z., Sukaiti E.K., M-Polynomial and Degree Based Topological Indices of Some Nanostructures. *Symmetry*, 2020, 12(5), 831-841.
- Shannon C.E., A mathematical theory of communication. *ACM SIGMOBILE Mob. Comput. Comm. Rev.*, 2001, 5(1), 3-55.
- Shirakol S., Kalyanshetti M., Hosamani S.M., QSPR analysis of certain distance based topological indices. *Appl. Math. Nonlinear Sci.*, 2019, 4(2), 371-386.
- Shirdel G.H., Rezapour H., Sayadi A.M., The hyper-Zagreb index of graph operations. *Iran. J. Math. Chem.*, 2013, 4(2), 213-220.

- Siddiqui M.K., Imran M., Ahmad A., On Zagreb indices, Zagreb polynomials of some nanostar dendrimers. *Appl. Math. Comput.*, 2016a, 280, 132-139.
- Siddiqui M.K., Naeem M., Rahman N.A., Imran M., Computing topological indices of certain networks. *J. Optoelect. Adv. Mater.*, 2016b, 18(September-October 2016), 884-892.
- Solé R.V., Valverde S. Information Theory of Complex Networks: On Evolution and Architectural Constraints. In: Ben-Naim E., Frauenfelder H., Toroczkai Z. (Eds.) *Complex Networks. Lecture Notes in Physics*, Vol. 650. Springer, Berlin, Heidelberg, 2004.
- Tan Y.J., Wu J., Network structure entropy and its application to scale-free networks. *Syst. Eng. Theory Practice*, 2004, 6(001).
- Trucco E., A note on the information content of graphs. *Bull. Math. Biophys.*, 1956, 18(2), 129-135.
- Ulanowicz R.E., Quantitative methods for ecological network analysis. *Comput. Biol. Chem.*, 2004, 28(5-6), 321-339.
- Wu W., Zhang C., Lin W., Chen Q., Guo X., Qian Y., et al., Quantitative structure-property relationship (QSPR) modeling of drug-loaded polymeric micelles via genetic function approximation. *PloS One*, 2015 10(3), 51-69.