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Degree Based Topological Indices of Vitamins

[1] Veena M G

[1] Assistant Professor, Department of Mathematics, Govt. First Grade College, Magadi, Karnataka, India
Corresponding Author Email: [1] veenamgprakash@gmail.com

Abstract— This article is mainly focused on calculating degree based topological indices of some vitamins by edge partition of graphs vitamin K and vitamin E by using First Zagreb index, Second Zagreb index, Harmonic index, Atom Bond Connectivity (ABC) index, Sum connectivity index, Sigma index and Albertson index.

Index Terms: Topological indices, Vitamin K, Vitamin E, Harmonic index, Atom Bond Connectivity index.

I. INTRODUCTION

Organic compounds like vitamins are very essential for human body to function well, a small quantity of vitamins are essential for body funtioning[1]. Vitamin K is a fat soluble vitam in it is very useful for many body functions such as blood coagulation, bone mineralization and insulin sensitization. It is also found in some foods and is also available as a dietary supplement [2].

Vitamin K plays a very important role in proper functioning of liver and prevents excessive bleeding and helps in cloting of blood. It is also important for healthy bones. Vitamin K gets stored in the liver, so that one can need not eat it every day like other vitamins [3][4].

Vitamin E is a fat soluble, it exists in several foods like vegetable oil, cereals, meat, poultry, eggs and fruits. This vitamin helps in proper funtioning of majority of organs. It also acts as an antioxidants [5][6]. Rich vitamin E foods are canola oil, olive oil, margarine, almonds and peanuts. Vitamin E is also available from meat, dairy, green leafy vegetables.

Topological index is a molecular descriptor it can be used to predict a perticular value of a graph. from this index one can analyze mathematical values and further investigate some physicochemical properties of a molecule [7].

Consider a simple connected graph G with vertices V is denoted as a set $v_1, v_2, v_3 \ldots\ldots\ldots v_n$ and edges E denoted as a set $e_1, e_2, e_3 \ldots\ldots e_n$ the degree of the vertex d_u is the number of neighbor vertices of G.

II. LITERATURE REVIEW

A. First and and second zagreb index:

The First Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$, are the first degree based topological indices invented by Gutman and Trinajsti in 1972and these indices are defined as[8].

$$M_1(G) = \sum_{u,v\varepsilon E(G)} (d_u + d_v)$$

$$M_2(G) = \sum_{u,v\varepsilon E(G)} (d_u * d_v)$$

B. Atom Bond Connectivity index:

One of the familear connectivity index is the Atom Bond connectivity (ABC) it was introduced by Estrada et.al [9] and is defined as

$$\mathrm{ABC}(G) = \sum_{u,v\varepsilon E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

C. Harmonic index:

In 1980's Siemion Fajtlowicz introduced a new topological indicator and named as Harmonic index and is defined as the weights $\frac{2}{d_u+d_v}$ of all edges u, v of G, where d_u denotes the degree of a vertex u in G[10].

$$H(G) = \sum_{u,v\varepsilon E(G)} \frac{2}{d_u + d_v}$$

D. Sum connectivity index:

The sum connectivity index was introduced by Nenad Trinajstic and Bo Zhou. It is defined as[11]

$$\mathrm{SCI}(G) = \sum_{u,v\varepsilon E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

E. Sigma index:

Amer et. Al introduced the Sigma index in 1900 which is defined as [12]

$$\sigma(G) = \sum_{u,v\varepsilon E(G)} (d_u - d_v)^2$$

F. Albertson index:

In 1997, the Albertson index of connected graph G, introduced by Albertson, is defined as,[13]

$$\mathrm{Alb}(G) = \sum_{u,v\varepsilon E(G)} |d_u - d_v|$$

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III. MAIN RESULTS

A. Topological indices of vitamine K($C_{31}H_{40}O_2$):

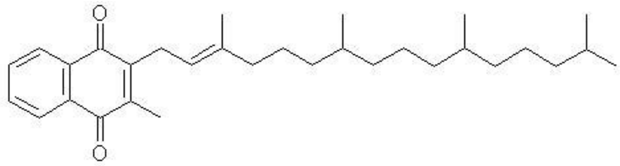

Fig. 1. Chemical structure of vitamin K ($C_{31}H_{40}O_2$)

From fig 1, the chemical structure of vitamin K $e_{i,j}$ denotes the edges connecting the vertices d_i *and* d_j. Two dimentional structure containing edges of the type

$e(2,2) = 10, e(3,3) = 6, e(2,3) = 10$ and $e(1,3) = 8$

Theorem 1: Prove the first and second Zagreb index of vitamin K ($C_{31}H_{40}O_2$) are $M_1(G) = 158$ *and* $M_2(G) = 178$

Proof: $M_1(G) = \sum_{u,v\varepsilon E(G)} (d_u + d_v)$

$= e(2,2).(2+2) + e(3,3).(3+3) + e(2,3).(2+3) + e(1,3).(1+3)$

=10(4) + 6(6) + 10(5) + 8(4)

=158

$$M_2(G) = \sum_{u,v\varepsilon E(G)} (d_u * d_v)$$

=e(2,2). (2*2) + e(3,3).(3*3) + e(2,3).(2*3) + e(1,3).(1*3)

=10(4) + 6(9) + 10(6) + 8(3)

=178

Theorem 2: The Atom bond connectivity index of vitamin K ($C_{31}H_{40}O_2$) is 25.5731

Proof: $ABC(G) = \sum_{u,v\varepsilon E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$

$=e(2,2).\sqrt{\frac{2+2-2}{2*2}} + e(3,3).\sqrt{\frac{3+3-2}{3*3}} + e(2,3).\sqrt{\frac{2+3-2}{2*3}} + e(1,3).\sqrt{\frac{1+3-2}{1*3}}$

=25.5731

Theorem 3: The Harmonic index of vitamin K ($C_{31}H_{40}O_2$) is 15

Proof: $H(G) = \sum_{u,v\varepsilon E(G)} \frac{2}{d_u+d_v}$

$=e(2,2).(\frac{2}{2+2})+e(3,3).(\frac{2}{3+3})+e(2,3).(\frac{2}{2+3})+e(1,3).(\frac{2}{1+3})$

=15

Theorem 4: The Sum connectivity index of vitamin K ($C_{31}H_{40}O_2$) is 16.4721

Proof: $SCI(G) = \sum_{u,v\varepsilon E(G)} \frac{1}{\sqrt{d_u+d_v}}$

$=e(2,2).(\frac{1}{\sqrt{2+2}}) + e(3,3).(\frac{1}{\sqrt{3+3}}) + e(2,3).(\frac{1}{\sqrt{2+3}}) + e(1,3).(\frac{1}{\sqrt{1+3}})$

=16.4721

Theorem 5: The sigma index of vitamin K ($C_{31}H_{40}O_2$) is 282

Proof: $\sigma(G) = \sum_{u,v\varepsilon E(G)} (d_u - d_v)^2$

$=e(2,2).(2-2)^2 + e(3,3).(3-3)^2 + e(2,3).(2-3)^2 + e(1,3).(1-3)^2$

=282

Theorem 6: The Albertson index of vitamin K ($C_{31}H_{40}O_2$) is 66

Proof: $Alb(G) = \sum_{u,v\varepsilon E(G)} |d_u - d_v|$

$=e(2,2).|2-2| + e(3,3).|3-3| + e(2,3).|2-3| + e(1,3).|1-3|$

= 66

B. Results of vitamin E

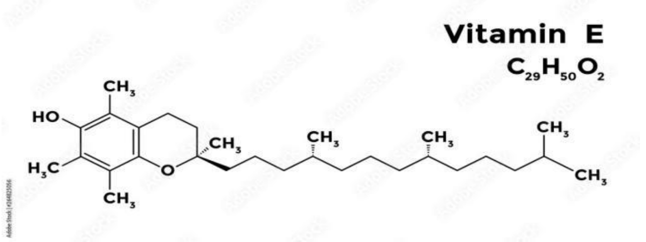

Fig. 2. Chemical structure of vitamin E

From the above structure of vitamin E let $e_{i,j}$ denotes the edges connecting the vertices d_i *and* d_j. Two dimentional structure containing edges of the type

$e(2,2) = 7, e(3,3) = 6, e(2,3) = 2, e(1,3) = 8, e(2,4) = 3$ and $e(1,4) = 1$

Theorem 1: The first and second Zagreb index of vitamin E($C_{29}H_{50}O_2$) are $M_1(G) = 129$ *and* $M_2(G) = 146$

Proof: $M_1(G) = \sum_{u,v\varepsilon E(G)} (d_u + d_v)$

$= e(2,2).(2+2) + e(3,3).(3+3) + e(2,3).(2+3) + e(1,3).(1+3) + e(1,4).(1+4) + e(2,4).(2+4)$

=7(4) + 6(6) + 2(5) + 8(4) + 1(5) + (6)

=129

$$M_2(G) = \sum_{u,v\varepsilon E(G)} (d_u * d_v)$$

=e(2,2).(2*2)+e(3,3).(3*3)+e(2,3).(2*3)+e(1,3).(1*3)+e(1,4).(1*4)+e(2,4).(2*4)

=7(4)+6(9)+2(6)+8(3)+1(4)+3(8)

=146

Theorem 2: The Atom bond connectivity index of vitamin E ($C_{29}H_{50}O_2$) is 19.8832

Proof: $ABC(G) = \sum_{u,v\varepsilon E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$

$=e(2,2).\sqrt{\frac{2+2-2}{2*2}} + e(3,3).\sqrt{\frac{3+3-2}{3*3}} + e(2,3).\sqrt{\frac{2+3-2}{2*3}} + e(1,3).\sqrt{\frac{1+3-2}{1*3}} + e(1,4).\sqrt{\frac{1+4-2}{1*4}} + e(2,4).\sqrt{\frac{2+4-2}{2*4}}$

= 19.8832

Theorem 3: The Harmonic index of vitamin E ($C_{29}H_{50}O_2$) is 12.9

Proof: $H(G) = \sum_{u,v\varepsilon E(G)} \frac{2}{d_u+d_v}$

$=e(2,2).(\frac{2}{2+2})+e(3,3).(\frac{2}{3+3})+e(2,3).(\frac{2}{2+3})+e(1,3).(\frac{2}{1+3})$

$+e(1,4).(\frac{2}{1+4})+e(2,4).(\frac{2}{2+4})$

=12.9

Theorem 4: The Sum connectivity index of vitamin E ($C_{29}H_{50}O_2$) is 11.2676

Proof: $SCI(G) = \sum_{u,v\varepsilon E(G)} \frac{1}{\sqrt{d_u+d_v}}$

[1]. = $\mathbf{e(2,2)}.(\frac{1}{\sqrt{2+2}}) + \mathbf{e(3,3)}.(\frac{1}{\sqrt{3+3}}) + \mathbf{e(2,3)}.(\frac{1}{\sqrt{2+3}}) + \mathbf{e(1,3)}.(\frac{1}{\sqrt{1+3}}) + \mathbf{e(1,4)}.(\frac{1}{\sqrt{1+3}}) + \mathbf{e(2,4)}.(\frac{1}{\sqrt{2+4}})$

=11.2676

Theorem 5: The sigma index of vitamin E ($C_{29}H_{50}O_2$) is 55

Proof: $\sigma(G) = \sum_{u,v\varepsilon E(G)} (d_u - d_v)^2$

= $e(2,2).(2-2)^2 + e(3,3).(3-3)^2 + e(2,3).(2-3)^2 + e(1,3).(1-3)^2 + e(1,4).(1-4)^2 + e(2,4).(2-4)^2$

=55

Theorem 6: The Albertson index of vitamin E ($C_{29}H_{50}O_2$) is 27

Proof: $Alb(G) = \sum_{u,v\varepsilon E(G)} |d_u - d_v|$

= $e(2,2).|2-2| + e(3,3).|3-3| + e(2,3).|2-3| + e(1,3).|1-3| + e(1,4).|1-4| + e(2,4).|2-4|$

= 27

IV. CONCLUSION

In this aricle we computed degree based topological indices of vitamins. These indices serve as a valuable tool for calculating physicochemical traits of drugs. These finding contribute significantly to our understanding of the mathematical aspects.

REFERENCES

[1] Lee, F. A., & Lee, F. A. (1983). The vitamins. Basic Food Chemistry, 199-224.

[2] Tsugawa, N. (2015). Cardiovascular diseases and fat soluble vitamins: vitamin D and vitamin K. Journal of nutritional science and vitaminology, 61(Supplement), S170-S172.

[3] Shearer, M. J., & Newman, P. (2008). Metabolism and cell biology of vitamin K. Thrombosis and haemostasis, 100(10), 530-547.

[4] Vermeer, C., Jie, K. S., & Knapen, M. H. J. (1995). Role of vitamin K in bone metabolism. Annual review of nutrition, 15(1), 1-21.

[5] Parker, A. L., Waddington, S. N., Nicol, C. G., Shayakhmetov, D. M., Buckley, S. M., Denby, L., ... & Baker, A. H. (2006). Multiple vitamin K-dependent coagulation zymogens promote adenovirus-mediated gene delivery to hepatocytes. Blood, 108(8), 2554-2561.

[6] Niki, E., & Traber, M. G. (2012). A history of vitamin E. Annals of Nutrition and Metabolism, 61(3), 207-212.

[7] Randić, M. (1991). Generalized molecular descriptors. Journal of Mathematical Chemistry, 7(1), 155-168.

[8] Réti, T. (2012). On the relationships between the first and second Zagreb indices. Match-Communications in Mathematical and Computer Chemistry, 68(1), 169.

[9] Das, K. C., Gutman, I., & Furtula, B. (2011). On atom-bond connectivity index. Chemical Physics Letters, 511(4-6), 452-454.

[10] Li, J., & Shiu, W. C. (2014). The harmonic index of a graph. The Rocky Mountain Journal of Mathematics, 44(5), 1607-1620.

[11] Lučić, B., Nikolić, S., Trinajstić, N., Zhou, B., & Turk, S. I. (2010). Sum-connectivity index. Novel Molecular Structure Descriptors-Theory and Applications I, 101-136.

[12] SEKAR, A., PRABHAVATHI, K., & RANJITHKUMAR, M. A. (2022). SIGMA INDEX IN SOME SPECIAL GRAPHS.

[13] Ünal, S. O. On Vertex-Degree-Based Indices of Monogenic Semigroup Graphs. Ikonion Journal of Mathematics, 4(2), 12-20.