Determination of Some Degree Based Topological Indices of Poly – L – Lysine (PLL) Dendrimer

Emily Jennifer. S, [1] Rajam. K, [2] Mary. U [3]

[1 & 2] Research Scholars, [3] Associate Professor, Department of Mathematics,

Nirmala College for Women, Coimbatore, India.

[1] emilyjennifer93@gmail.com; [2] rajee.mat@gmail.com;

[3] marycbe@gmail.com.

ABSTRACT:

In hypothetical science, the chemical compounds are displayed as graphs where every vertex is represented as atoms and the edges between the atoms represents the covalent bonds. Therefore, they are known as molecular graph. In this paper, we compute Randić index, Sum connectivity index, Harmonic index and Forgotten topological index of Poly – L – Lysine (PLL) dendrimer.

KEYWORDS:

Forgotten topological index, Harmonic index, Poly – L – Lysine (PLL) Dendrimer, Randić index, Sum connectivity index.

I. INTRODUCTION:

Dendrimer science was first found by Fritz Vögtle and colleagues in 1978. Dendrimers are profoundly branched and receptive three – dimensional macromolecules, with progressive layers of branching units encompassing a focal centre. They are being explored for potential uses in science, nanotechnology, quality treatment, sedate conveyance, photonics and different fields. Chemical graph theory is a significant instrument for considering atomic structures. In hypothetical chemistry, molecular descriptors, especially topological indices are utilized for displaying data of particles, including physical, pharmacological and organic of chemical compounds.

Lysines (symbol Lys or K) is an α – amino acid which is used in the biosynthesis of proteins. It contains α – amino group, an α – carboxylic acid group and a side chain lysyl. Polylysine refers to a few sorts of lysine homopolymers which may contrast from one another as far as stereochemistry and connection position. The forerunner amino acid lysine contains two amino groups, one at the α – carbon and one at the ε – carbon. Either can be the area of polymerization, which results in α – polylysine or ε – polylysine. α – polylysine is a manufactured polymer which can be made out of either L – lysine or D – lysine. “L” and “D” refers to the chirality at lysine’s focal carbon. This outcomes in Poly – L – Lysine (PLL) and Poly – D – Lysine (PDL) respectively.

In the year 1975, Milan Randić introduced Randić index [6] which is defined for the graph G,

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Where d_u and d_v is the degree of the vertices u and v respectively.

Sum connectivity index was introduced by Zhou and Trinjstic [8]. For the graph G, it is defined as,

$$S(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

Further they are determined for Dutch Windmill graph by Rajesh Kanna. M. R et. al. [5].

In 1987, Fajtlowicz [2] introduced Harmonic index which is another variant of Randić connectivity index. For a graph G, harmonic index is defined as,

$$H(G) = \sum_{uv\in E(G)} \frac{1}{d(u) + d(v)}$$

The forgotten topological index was introduced by Furtula and Gutman [3] which is also called as F – index and for a graph G, it is defined as,

$$F(G) = \sum_{u\in V(G)} (d(u))^3 = \sum_{uv\in E(G)} [(d(u))^2 + (d(v))^2]$$

Figure (1.1), represents the third generation of Poly – L – Lysine (PLL) dendrimer.

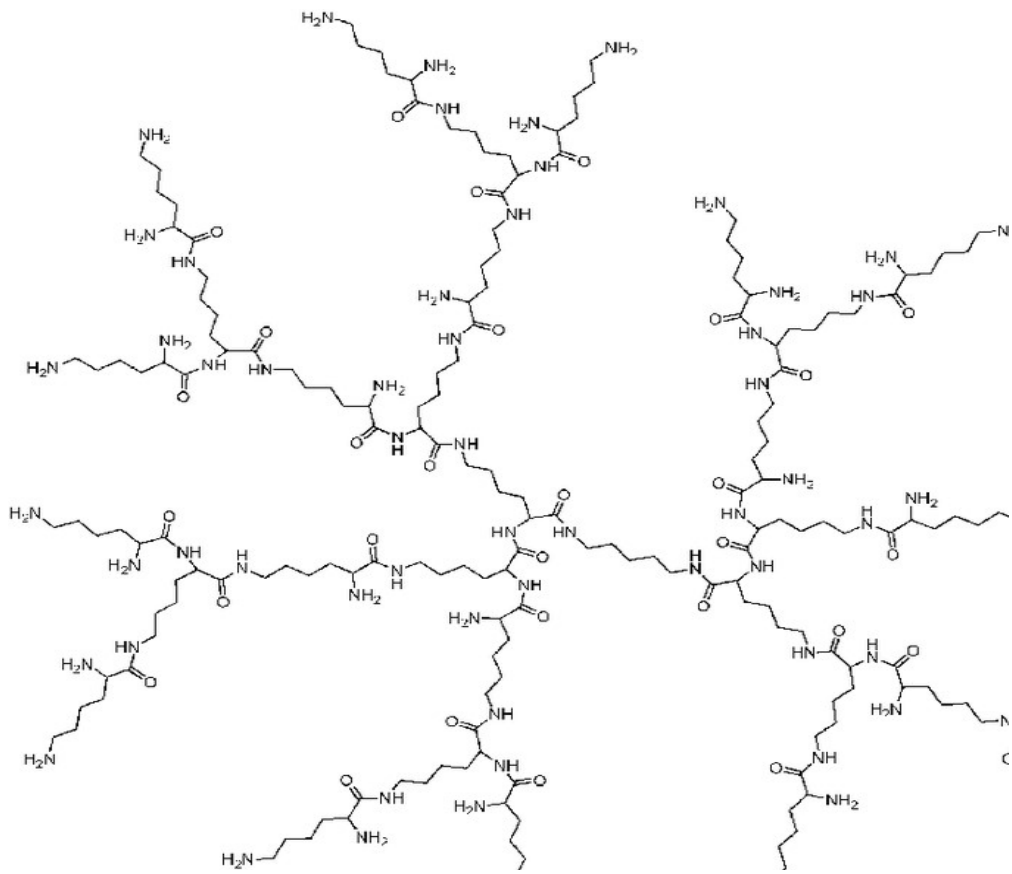

Fig. 1 Third generation of PLL dendrimer

II. STRUCTURAL PROPERTIES:

The Poly – L – Lysine (PLL) dendrimer graph can be represented as $(DPLL)_n$ where 'n' represents the number of generations of the dendrimer.

The order of $(DPLL)_n$ is given by,

$|V[(DPLL)_n]| = 7 + 3^4.2^{n-1} + 9\sum_{i=3}^{n} 2^{i-2}$; if n ≥ 3.

The size of $(DPLL)_n$ is given by,

$|E[(DPLL)_n]| = 6 + 3^4.2^{n-1} + 9\sum_{i=3}^{n} 2^{i-2}$; if n ≥ 3.

The following table (2.1) illustrates the partition of edges of the $(DPLL)_n$ graph based on end vertices of each edge. The edge type is $E_{(d_u,d_v)}$ where uv ∈ E[$(DPLL)_n$].

TABLE I

EDGE PARTITION OF $(DPLL)_n$ GRAPH

$E_{(d_u,d_v)}$	NUMBER OF EDGES FOR n ≥ 3
$E_{(1,2)}$	2^{n+1}
$E_{(1,3)}$	$15.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})$
$E_{(2,2)}$	$32.2^{n-1} + 8\sum_{i=3}^{n}(2^{i-3}) + 6$
$E_{(2,3)}$	$21.2^{n-1} + 6\sum_{i=3}^{n}(2^{i-3})$

$E_{(3,3)}$	$9.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})$

III. MAIN RESULTS:

Theorem 3.1: Consider a $(DPLL)_n$ graph then the Randić index is,

$$\chi[(DPLL)_n] = \left\{2^{n-1}\left[\frac{4\sqrt{2}+10\sqrt{3}+7\sqrt{6}+38}{2}\right] + \sum_{i=3}^{n}(2^{i-3})\left[\frac{2\sqrt{3}+3\sqrt{6}+14}{3}\right] + 3 \text{ ; if } n \geq 3.\right.$$

Proof:

By the definition of Randić index and the values from the table (2.1), we get,

$$\chi[(DPLL)_n] = |E_{(1,2)}| \sum_{uv\in E_{(1,2)}[(DPLL)_n]} \frac{1}{\sqrt{d_u d_v}} + |E_{(1,3)}| \sum_{uv\in E_{(1,3)}[(DPLL)_n]} \frac{1}{\sqrt{d_u d_v}} + |E_{(2,2)}| \sum_{uv\in E_{(2,2)}[(DPLL)_n]} \frac{1}{\sqrt{d_u d_v}} + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}[(DPLL)_n]} \frac{1}{\sqrt{d_u d_v}} + |E_{(3,3)}| \sum_{uv\in E_{(3,3)}[(DPLL)_n]} \frac{1}{\sqrt{d_u d_v}}$$

$$= \left[2^{n+1}\frac{1}{\sqrt{1.2}}\right] + \left[15.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})\left(\frac{1}{\sqrt{1.3}}\right)\right] + \left[32.2^{n-1} + 8\sum_{i=3}^{n}\left((2^{i-3})+6\right)\left(\frac{1}{\sqrt{2.2}}\right)\right] + \left[21.2^{n-1} + 6\sum_{i=3}^{n}(2^{i-3})\left(\frac{1}{\sqrt{2.3}}\right)\right] + \left[9.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})\left(\frac{1}{\sqrt{3.3}}\right)\right]$$

$$\chi[(DPLL)_n] = 2^{n-1}\left[\frac{4\sqrt{2}+10\sqrt{3}+7\sqrt{6}+38}{2}\right] + \sum_{i=3}^{n}(2^{i-3})\left[\frac{2\sqrt{3}+3\sqrt{6}+14}{3}\right] + 3.$$

Remark 3.1.1: The Randić index of $(DPLL)_n$ graph,

When n = 1, $\chi(G_1) = \frac{6\sqrt{2}+10\sqrt{3}+7\sqrt{6}+45}{3}$.

When n = 2, $\chi(G_2) = 4\sqrt{2} + 10\sqrt{3} + 7\sqrt{6} + 41$.

Theorem 3.2: Consider a $(DPLL)_n$ graph then the Sum connectivity index is,

$$S[(DPLL)_n] = \left\{2^{n-1}\left[\frac{40\sqrt{3}+126\sqrt{5}+45\sqrt{6}+705}{30}\right] + \sum_{i=3}^{n}(2^{i-3})\left[\frac{18\sqrt{5}+5\sqrt{6}+75}{15}\right] + 3 \text{ ; if } n \geq 3.\right.$$

Proof:

$$S[(DPLL)_n] = |E_{(1,2)}| \sum_{uv\in E_{(1,2)}[(DPLL)_n]} \frac{1}{\sqrt{d_u+d_v}} + |E_{(1,3)}| \sum_{uv\in E_{(1,3)}[(DPLL)_n]} \frac{1}{\sqrt{d_u+d_v}} + |E_{(2,2)}| \sum_{uv\in E_{(2,2)}[(DPLL)_n]} \frac{1}{\sqrt{d_u+d_v}} + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}[(DPLL)_n]} \frac{1}{\sqrt{d_u+d_v}} + |E_{(3,3)}| \sum_{uv\in E_{(3,3)}[(DPLL)_n]} \frac{1}{\sqrt{d_u+d_v}}$$

$$= \left[2^{n+1}\frac{1}{\sqrt{1+2}}\right] + \left[15.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})\left(\frac{1}{\sqrt{1+3}}\right)\right] + \left[32.2^{n-1} + 8\sum_{i=3}^{n}\left((2^{i-3})+6\right)\left(\frac{1}{\sqrt{2+2}}\right)\right] + \left[21.2^{n-1} + 6\sum_{i=3}^{n}(2^{i-3})\left(\frac{1}{\sqrt{2+3}}\right)\right] + \left[9.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})\left(\frac{1}{\sqrt{3+3}}\right)\right]$$

$S[(DPLL)_n] = 2^{n-1}\left[\frac{40\sqrt{3}+126\sqrt{5}+45\sqrt{6}+705}{30}\right] + \sum_{i=3}^{n}(2^{i-3})\left[\frac{18\sqrt{5}+5\sqrt{6}+75}{15}\right] + 3.$

Remark 3.2.1: The Sum connectivity index of $(DPLL)_n$ graph,

When n = 1, $S(G_1) = \frac{20\sqrt{3}+42\sqrt{5}+15\sqrt{6}+270}{15}$.

When n = 2, $S(G_2) = \frac{40\sqrt{3}+126\sqrt{5}+45\sqrt{6}+75}{15}$.

Theorem 3.3: Consider a $(DPLL)_n$ graph then the Harmonic index is,

$H[(DPLL)_n] = \{2^{n-1}\left[\frac{1127}{30}\right] + \sum_{i=3}^{n}(2^{i-3})\left[\frac{121}{15}\right] + 3$; if $n \geq 3$.

Proof:

$$H[(DPLL)_n] = |E_{(1,2)}| \sum_{uv\in E_{(1,2)}[(DPLL)_n]} \frac{2}{d_u+d_v} + |E_{(1,3)}| \sum_{uv\in E_{(1,3)}[(DPLL)_n]} \frac{2}{d_u+d_v} + |E_{(2,2)}| \sum_{uv\in E_{(2,2)}[(DPLL)_n]} \frac{2}{d_u+d_v} + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}[(DPLL)_n]} \frac{2}{d_u+d_v} + |E_{(3,3)}| \sum_{uv\in E_{(3,3)}[(DPLL)_n]} \frac{2}{d_u+d_v}$$

$$= \left[2^{n+1}\frac{2}{1+2}\right] + \left[15.2^{n-1} + 2\sum_{i=3}^{n}(2^{i-3})\left(\frac{2}{1+3}\right)\right] + \left[32.2^{n-1} + 8\sum_{i=3}^{n}\left((2^{i-3})+6\right)\left(\frac{2}{2+2}\right)\right] + \left[21.2^{n-1} + 6\sum_{i=3}^{n}(2^{i-3})\left(\frac{2}{2+3}\right)\right]$$

$$+ \left[9.2^{n-1} + 2 \sum_{i=3}^{n} (2^{i-3}) \left(\frac{2}{3+3} \right) \right]$$

$H[(DPLL)_n] = 2^{n-1} \left[\frac{1127}{30}\right] + \sum_{i=3}^{n} (2^{i-3}) \left[\frac{121}{15}\right] + 3.$

Remark 3.3.1: The Harmonic index of $(DPLL)_n$ graph,

When n = 1, $H(G_1) = \frac{424}{15}$.

When n = 2, $H(G_2) = \frac{1172}{15}$.

Theorem 3.4: Consider a $(DPLL)_n$ graph then the forgotten topological index is,

$F[(DPLL)_n] = \{861.2^{n-1} + 198. \sum_{i=3}^{n} (2^{i-3}) + 48$; if n ≥ 3.

Proof:

$$F[(DPLL)_n] = |E_{(1,2)}| \sum_{uv \in E_{(1,2)}[(DPLL)_n]} [(d(u))^2 + (d(v))^2] + |E_{(1,3)}| \sum_{uv \in E_{(1,3)}[(DPLL)_n]} [(d(u))^2 + (d(v))^2] + |E_{(2,2)}| \sum_{uv \in E_{(2,2)}[(DPLL)_n]} [(d(u))^2 + (d(v))^2] + |E_{(2,3)}| \sum_{uv \in E_{(2,3)}[(DPLL)_n]} [(d(u))^2 + (d(v))^2] + |E_{(3,3)}| \sum_{uv \in E_{(3,3)}[(DPLL)_n]} [(d(u))^2 + (d(v))^2]$$

$$= [2^{n+1}((1)^2 + (2)^2)] + \left[15.2^{n-1} + 2 \sum_{i=3}^{n} (2^{i-3})((1)^2 + (3)^2) \right]$$

$$+ \left[32.2^{n-1} + 8 \sum_{i=3}^{n} \left((2^{i-3}) + 6 \right) ((2)^2 + (2)^2) \right]$$

$$+ \left[21.2^{n-1} + 6 \sum_{i=3}^{n} (2^{i-3})((2)^2 + (3)^2) \right]$$

$$+ \left[9.2^{n-1} + 2 \sum_{i=3}^{n} (2^{i-3})((3)^2 + (3)^2) \right]$$

$F[(DPLL)_n] = 861.2^{n-1} + 198. \sum_{i=3}^{n} (2^{i-3}) + 48.$

Remark 3.4.1: The Forgotten topological index of $(DPLL)_n$ graph,

When n = 1, $F(G_1) = 618$.

When n = 2, $F(G_2) = 1770$.

III. CONCLUSION:

In this paper, we studied some degree based topological indices of Poly – L – Lysine (PLL) dendrimer. These hypothetical outcomes are used in nanoscience, science, drugs and different fields that has a wide application prospect.

REFERENCES:

[1] Bondy. J. A and Murty. U. S. R, (2008), "*Graph Theory and its Applications*", Springer.
[2] Fajtlowicz. S, (1987), "*On conjectures of Graffiti - II*", Congressus Numerantium, Vol. 60, 187 – 197.
[3] Furtula. B and Gutman. I, (2015), "*A Forgotten Topological Index*" Journal of Mathematical Chemistry, Vol. 53, 1184 – 1190.
[4] Harary. F, (1969), "*Graph Theory*", Addison – Wesley, Reading, MA.

[5] Kanna. M. R. R, Kumar. R. P and Jagadeesh. R, (2016), "*Computation of Topological Indices of Dutch Windmill Graph*", Open Journal of Discrete Mathematics, Vol. 6, 74 – 81.

[6] Randić. M, (1975), "*On Characterization of Molecular Branching*", Journal of the American Chemical Society, Vol. 97, 6609 – 6615.

[7] Trinajstić. N, (1992), "*Chemical Graph Theory*", CRC Press, Boca Raton, FL.

[8] Zhou. B and Trinajstić. N, (2009), "*On a Novel Connectivity Index*", Journal of Mathematical Chemistry, Vol. 46, 1252 – 1270.