REVERSE DEGREE-BASED TOPOLOGICAL DESCRIPTORS OF CHIRAL PAMAM DENDRIMER

Akhila S[1*], D. Antony Xavier[2], Theertha Nair[3], Eddith Sarah Varghese[4], Annmaria Baby[5]

Article History: Received: 11.03.2023 **Revised:** 30.04.2023 **Accepted:** 27.06.2023

Abstract

Dendrimers have unique structures, a wide range of properties and extensive application in chemistry, thus it obtaining much attention in many disciplines. In the context of delivery and design of drugs, dendrimer serves as a catalyst. The relationship between the structure and properties of chemical compounds are analysed using the topological descriptor. A graphical representation of the molecular descriptor is plotted by numerical results of chiral PAMAM dendrimer and compared with each index.

Keywords: Nanoparticle, Dendrimer, Reverse index.

[1,2,3,4,5]Department of Mathematics, Loyola College (Affiliated to the University of Madras), Chennai, India.

Corresponding Email: [1*]akilsuresh0712@gmail.com

DOI: 10.31838/ecb/2023.12.s3.554

1. Introduction

Scientists from chemistry, chemical engineering and medicine are working together to develop nanoparticles that enables drug delivery. A polymer has become the forerunner in the chase to discover the ideal carrier, due to their adaptability and deliver the drug to specific parts of the body. Using covalent conjugation, it is possible to deliver drug molecules across the cell membrane in a targeted manner (for example, against cancer cells using folic acid). A unique structure, dendrimers are developed by Vogtle and his co-workers in 1978. Dendrimer are hyper branched polymer materials with single molecular weight. A dendrimer contains a single core, and various interior layers composed of iterating units and active amine groups at the end. The extension of dendrimer is predictable even though they have a branching architecture. Dendrimers are generated in two methods: divergent method, starts from the core and develop the generation and convergent method, synthesis from surface and ends at the core. Because of a unique characteristic of dendrimers such as unimolecular micelles, polyvalency, electrostatic inter-actions, it is a great carrier in nanomedicine field. In gene delivery system dendrimer plays a vital role due to its high functionality [1].

In graph theory, the chemical compounds are described as graphs where atoms are defined as vertices and bonds are indicated as edges. Cheminformatics is a unification of mathematics and medicinal chemistry. In medicinal chemistry, it is critical to know the properties of the drugs, in order to track the process and operational efficiency. A topological index describes a physicochemical property of compounds. In QSAR/QSPRs study, the properties of molecular structures such as photochemical, pharmacologic, pharmacodynamic and pharmacogenomics are evaluated by structural characterisation. The molecular properties namely boiling point, flash point, molar refraction, critical pressure, osmotic coefficients, polarizability etc., can be evaluated by topological indices [2, 3]. Topological indices can therefore be used to quantitatively analyse and understand different chemical structures and chemical networks [4]. Thus, topological indices enable to evaluate and compute the chemical structure and its networks in more detail.

PAMAM structures have both light-emitting and electrodeposition properties due to their achiral and hydrophobic surfaces [5]. As shown in Figure 1, the core of Chiral PAMAM dendrimer is tetracarboxylic, with four branches used in nano catalysis [6]. Chiral PAMAM dendrimer's n^{th} generation is denoted as CD_n: $n \leq 1$. The reverse degree-based topological descriptor for CD_n can be determined. We suggest the readers to refer [7, 8, 9, 10] for recent papers in reverse topological indices.

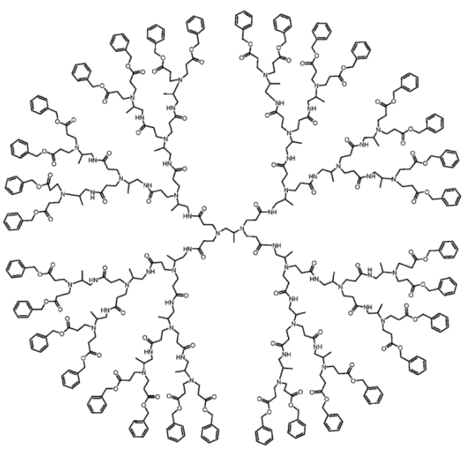

Figure 1: The molecular structure of Chiral PAMAM dendrimer with generation 3.

2. Mathematical Terminologies

Let $\delta = (\mathbb{V}, \mathbb{E})$ where $\mathbb{V}$ indicates the set of vertices and $\mathbb{E}$ represent the set of edges respectively. Let $\zeta \in \mathbb{V}(\delta)$, then the degree of ζ is the number of edges incident to the vertex ζ, denoted as Γ_{ζ}. Kulli [11] introduced the concept, reverse vertex degree $(\mathcal{R}(\zeta))$ defined as: $\mathcal{R}(\zeta) = 1 - \Gamma(\zeta) + \Delta(\delta)$, where Δ is the highest degree in a graph. As result of randic degree-based indices, introduced by Milan Randic [12] and its reverse Randic index can be stated as follows:

$$\mathcal{R}\mathrm{R}_{\alpha}(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} (\mathcal{R}(\zeta) \times \mathcal{R}(\xi))^{\alpha}, \qquad \alpha = \frac{1}{2}, -\frac{1}{2}, 1, -1$$

Atom bond connectivity (ABC) index was introduced by Estrada et al. [13] and its reverse is presented as:

$$\mathcal{R}\mathrm{ABC}(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} \sqrt{\frac{\left(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\right) - 2}{(\mathcal{R}(\zeta) \times \mathcal{R}(\xi))}}$$

Geometric arithmetic (GA) index was presented by Vukicevic and Furtula in [14], whose reverse index as:

$$\mathcal{R}\mathrm{GA}(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} \frac{2\sqrt{(\mathcal{R}(\zeta) \times \mathcal{R}(\xi))}}{(\mathcal{R}(\zeta) + \mathcal{R}(\xi))}$$

Gutman et al. [15, 16] introduced the first and second Zagreb indices and the reverse first Zagreb index and the reverse second Zagreb index is defined as:

$$\mathcal{R}\mathrm{M}_1(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} \left(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\right)$$

$$\mathcal{R}\mathrm{M}_2(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} \left(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\right)$$

A hyper Zagreb (HM) index was presented by shirdel et al. in [17] and its reverse is defined as:

$$\mathcal{R}\mathrm{HM}(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} (\mathcal{R}(\zeta) + \mathcal{R}(\xi))^2$$

Furtula and Gutman [18] presented the forgotten index and the reverse forgotten index is given as:

$$\mathcal{R}\mathrm{F}(\delta) = \sum_{\zeta\xi \in \mathrm{E}(\delta)} (\mathcal{R}(\zeta)^2 + \mathcal{R}(\xi)^2)$$

Furtula et al. introduced augumented Zagreb index in [19] and its reverse index as:

$$\mathcal{R}\mathrm{AZI}(\delta) = \sum_{\zeta\xi \in \mathrm{E}(\delta)} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi) - 2}\right)^3$$

First redefined, second redefined and third redefined Zagreb indices was introduced by Ranjini et al. [20] and the reverse first redefined, reverse second redefined and reverse third redefined Zagreb indices is given as:

$$\mathcal{R}\mathrm{ReZG}_1(\delta) = \sum_{\zeta\xi \in \mathrm{E}(\delta)} \left(\frac{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}\right)$$

$$\mathcal{R}\mathrm{ReZG}_2(\delta) = \sum_{\zeta\xi \in \mathrm{E}(\delta)} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}\right)$$

$$\mathcal{R}\mathrm{ReZG}_2(\delta) = \sum_{\zeta\xi \in \mathrm{E}(\delta)} \big(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\big)\big(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\big)$$

3. Results For Chiral Pamam Dendrimer

Let Chiral PAMAM dendrimer be the chemical graph, $\zeta = \mathrm{CD_n}$ has $42 \times 2^{n+1} - 31$ vertices and $22 \times 2^{n+2} - 32$ edges [6]. In $\mathrm{CD_n}$, degree for $5 \times 2^{n+2} - 91$ vertices, degree 2 for $13 \times 2^{n+2} - 15$ vertices and degree 1 for $6 \times 2^{n+1} - 7$ vertices. The vertex set of $\mathrm{CD_n}$ is given in Table 1. From Figure 2, four classes of edge partition are obtained by considering the degree of the end vertices. $20\times 2^{n+1} - 14$ edges $\zeta\xi$, where $\Gamma_\zeta = 3$ and $\Gamma_\xi = 2$ contained in the first edge partition. $16\times 2^{n+1} - 8$ edges $\zeta\xi$, where $\Gamma_\zeta = 2$ and $\Gamma_\xi = 2$ are in the second edge partition. $2^{n+2} - 3$ edges $\zeta\xi$, where $\Gamma_\zeta = 3$ and $\Gamma_\xi = 3$ contained in the third edge partition and $6\times 2^{n+1} - 7$ edges $\zeta\xi$, where $\Gamma_\zeta = 3$ and $\Gamma_\xi = 1$ contained in the fourth edge partition.

$$\mathfrak{E}'_{\zeta\xi} = \{(\Gamma_\zeta, \Gamma_\xi) |\ \zeta\xi \in \mathbb{E}(\delta)\}$$

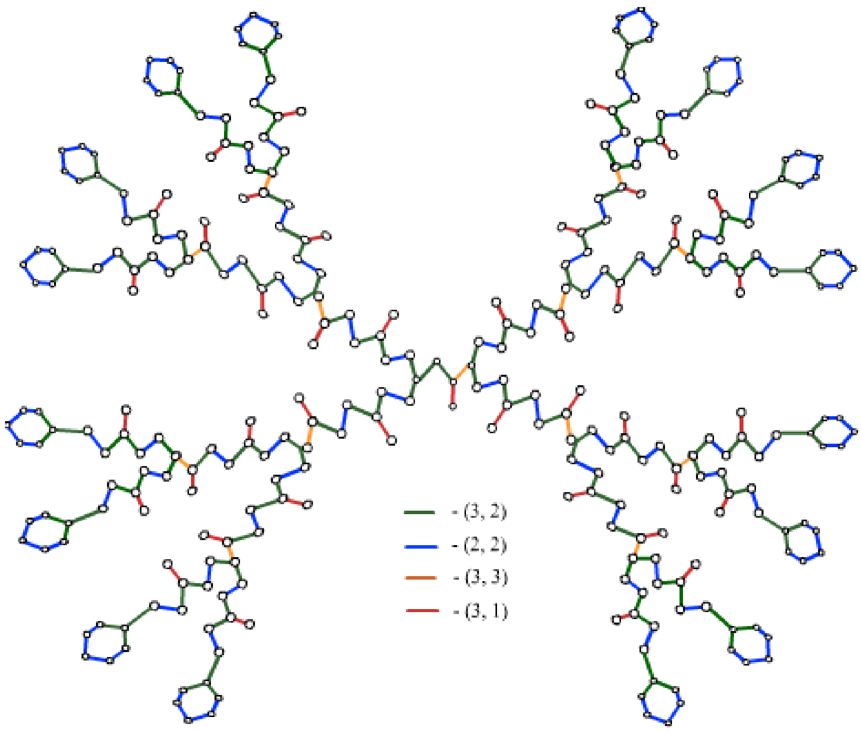

Figure 2: Edge partition of chiral PAMAM dendrimer, CD_2.

Γ_ζ	3	2	1
$\lvert\Gamma_\zeta\rvert$	$5 \times 2^{n+2} - 9$	$13 \times 2^{n+2} - 15$	$6 \times 2^{n+1} - 7$

Table 1: Vertex set of chiral PAMAM dendrimer CD_n

$\mathfrak{E}'_{\zeta\xi}$	$\lvert\mathfrak{E}'_{\zeta\xi}\rvert$	Set of edges
(3,2)	$20 \times 2^{n+1} - 14$	$\mathfrak{E}'_{3,2}$
(2,2)	$16 \times 2^{n+1} - 8$	$\mathfrak{E}'_{2,2}$
(3,3)	$2^{n+1} - 3$	$\mathfrak{E}'_{3,3}$
(3,1)	$6 \times 2^{n+1} - 7$	$\mathfrak{E}'_{3,1}$

Table 2: Edge partition of CD_n based on degree nodes

$\chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}$	$\lvert\mathfrak{E}'_{\zeta\xi}\rvert$	Set of edges
(1,2)	$20 \times 2^{n+1} - 14$	$\chi_{1,2}$
(2,2)	$16 \times 2^{n+1} - 8$	$\chi_{2,2}$
(1,1)	$2^{n+1} - 3$	$\chi_{1,1}$
(1,3)	$6 \times 2^{n+1} - 7$	$\chi_{1,3}$

Table 3: Reverse degree-based edge partition of CD_n

In Table 2, the edge partition based on the end vertices degree is given. In CD_n the maximum degree is 3. Based on the reverse vertex degree definition, $\mathcal{R}(\zeta) = 1 - \Gamma(\zeta) + \Delta(\delta)$. Table 3 shows the reverse degree-based edge partition of CD_n.

$$\chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)} = \{(\mathcal{R}(\zeta), \mathcal{R}(\xi)) \mid \zeta\xi \in \mathbb{E}(\delta)\}$$

Reverse general Randic index

$$\mathcal{R}\mathrm{R}_{\alpha}(\delta) = \sum_{\zeta\xi\in \mathrm{E}(\delta)} (\mathcal{R}(\zeta) \times \mathcal{R}(\xi))^{\alpha}, \qquad \alpha = \frac{1}{2}, -\frac{1}{2}, 1, -1$$

$\alpha = \frac{1}{2};$

$$\mathcal{R}\mathrm{R}_{\frac{1}{2}}(\delta) = \sum_{\zeta\xi\in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\right)^{\frac{1}{2}}$$

$$= \sum\nolimits_{\zeta\xi\in \chi_{1,2}} \sqrt{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)} + \sum\nolimits_{\zeta\xi\in \chi_{2,2}} \sqrt{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)} + \sum\nolimits_{\zeta\xi\in \chi_{1,1}} \sqrt{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)} + \sum\nolimits_{\zeta\xi\in \chi_{1,3}} \sqrt{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}$$

$$= \sqrt{2}(20 \times 2^{n+1} - 14) + 2(16 \times 2^{n+1} - 8) + 2^{n+1} - 3 + \sqrt{3}(6 \times 2^{n+1} - 7)$$

$$= 40\sqrt{2} \times 2^{n} - 7\sqrt{3} - 14\sqrt{2} + 12\sqrt{3} \times 2^{n} + 68 \times 2^{n} - 19$$

$\alpha = -\frac{1}{2};$

$$\mathcal{R}\mathrm{R}_{\frac{-1}{2}}(\delta) = \sum_{\zeta\xi\in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\right)^{\frac{-1}{2}}$$

$$= \sum\nolimits_{\zeta\xi\in \chi_{1,2}} \frac{1}{\sqrt{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}} + \sum\nolimits_{\zeta\xi\in \chi_{2,2}} \frac{1}{\sqrt{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}} + \sum\nolimits_{\zeta\xi\in \chi_{1,1}} \frac{1}{\sqrt{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}} + \sum\nolimits_{\zeta\xi\in \chi_{1,3}} \frac{1}{\sqrt{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}}$$

$$= \frac{1}{\sqrt{2}}(20 \times 2^{n+1} - 14) + \frac{1}{2}(16 \times 2^{n+1} - 8) + 2^{n+1} - 3 + \frac{1}{\sqrt{3}}(6 \times 2^{n+1} - 7)$$

$$= 20\sqrt{2} \times 2^{n} - \frac{7\sqrt{3}}{3} - 7\sqrt{2} + 4\sqrt{3} \times 2^{n} + 20 \times 2^{n} - 7$$

$\alpha = 1;$

$$\mathcal{R}\mathrm{R}_{1}(\delta) = \sum_{\zeta\xi\in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\right)^{1}$$

$$= \sum\nolimits_{\zeta\xi\in \chi_{1,2}} (\mathcal{R}(\zeta) \times \mathcal{R}(\xi)) + \sum\nolimits_{\zeta\xi\in \chi_{2,2}} (\mathcal{R}(\zeta) \times \mathcal{R}(\xi)) + \sum\nolimits_{\zeta\xi\in \chi_{1,1}} (\mathcal{R}(\zeta) \times \mathcal{R}(\xi)) + \sum\nolimits_{\zeta\xi\in \chi_{1,3}} (\mathcal{R}(\zeta) \times \mathcal{R}(\xi))$$

$$= 2(20 \times 2^{n+1} - 14) + 4(16 \times 2^{n+1} - 8) + 2^{n+1} - 3 + 3(6 \times 2^{n+1} - 7)$$

$$= 62 \times 2^{n+2} - 84$$

$\alpha = -1;$

$$\mathcal{R}\mathrm{R}_{-1}(\delta) = \sum_{\zeta\xi\in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\right)^{-1}$$

$$= \sum\nolimits_{\zeta\xi\in \chi_{1,2}} \frac{1}{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)} + \sum\nolimits_{\zeta\xi\in \chi_{2,2}} \frac{1}{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)} + \sum\nolimits_{\zeta\xi\in \chi_{1,1}} \frac{1}{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)} + \sum\nolimits_{\zeta\xi\in \chi_{1,3}} \frac{1}{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}$$

$$= \frac{1}{2}(20 \times 2^{n+1} - 14) + \frac{1}{4}(16 \times 2^{n+1} - 8) + 2^{n+1} - 3 + \frac{1}{3}(6 \times 2^{n+1} - 7)$$

$$= 9 \times 2^{n+2} - \frac{43}{3}$$

Reverse Atom Bond Connectivity Index

$$\mathcal{R}\mathrm{ABC}(\delta) = \sum_{\zeta\xi\in\chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \sqrt{\frac{\big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big)-2}{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}}$$

$=\sum_{\zeta\xi\in\chi_{1,2}} \sqrt{\frac{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))-2}{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}} + \sum_{\zeta\xi\in\chi_{2,2}} \sqrt{\frac{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))-2}{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}} + \sum_{\zeta\xi\in\chi_{1,1}} \sqrt{\frac{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))-2}{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}} +$
$\sum_{\zeta\xi\in\chi_{1,3}} \sqrt{\frac{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))-2}{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}}$
$= \frac{1}{\sqrt{2}}(20\times 2^{n+1}-14) + \frac{1}{\sqrt{2}}(16\times 2^{n+1}-8) + 2^{n+1} - 3 + \frac{\sqrt{2}}{\sqrt{3}}(6\times 2^{n+1}-7)$
$= 36\sqrt{2}\times 2^{n} - \frac{7\sqrt{6}}{3} - 11\sqrt{2} + 4\sqrt{6}\times 2^{n}$

Reverse Geometric Arithmetic Index

$$\mathcal{R}\mathrm{GA}(\delta) = \sum_{\zeta\xi\in\chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \frac{2\sqrt{\big(\mathcal{R}(\zeta)\times\mathcal{R}(\xi)\big)}}{\big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big)}$$

$=$
$\sum_{\zeta\xi\in\chi_{1,2}} \frac{2\sqrt{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}}{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))} + \sum_{\zeta\xi\in\chi_{2,2}} \frac{2\sqrt{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}}{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))} + \sum_{\zeta\xi\in\chi_{1,1}} \frac{2\sqrt{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}}{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))} + \sum_{\zeta\xi\in\chi_{1,3}} \frac{2\sqrt{(\mathcal{R}(\zeta)\times\mathcal{R}(\xi))}}{(\mathcal{R}(\zeta)+\mathcal{R}(\xi))}$
$= \frac{2\sqrt{2}}{3}(20\times 2^{n+1}-14) + (16\times 2^{n+1}-8) + 2^{n+1} - 3 + \frac{\sqrt{3}}{2}(6\times 2^{n+1}-7)$
$= 9\times 2^{n+2} + \frac{\sqrt{3}}{2}(6\times 2^{n+1}-7) + \frac{2\sqrt{2}}{3}(20\times 2^{n+1}-14) - 11$

Reverse First Zagreb Index

$$\mathcal{R}\mathrm{M}_1(\delta) = \sum_{\zeta\xi\in\chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big)$$

$= \sum_{\zeta\xi\in\chi_{1,2}} \big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big) + \sum_{\zeta\xi\in\chi_{2,2}} \big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big) + \sum_{\zeta\xi\in\chi_{1,2}} \big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big)$
$+ \sum_{\zeta\xi\in\chi_{1,2}} \big(\mathcal{R}(\zeta)+\mathcal{R}(\xi)\big)$
$= 3(20\times 2^{n+1}-14) + 4(16\times 2^{n+1}-8) + 2(2^{n+1}-3) + 4(6\times 2^{n+1}-7)$
$= 76\times 2^{n+2} - 108$

Reverse Second Zagreb Index

$$\mathcal{R}\mathrm{M}_2(\delta) = \sum_{\zeta\xi\in\chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \big(\mathcal{R}(\zeta)\times\mathcal{R}(\xi)\big)$$

$= \sum_{\zeta\xi\in\chi_{1,2}} \big(\mathcal{R}(\zeta)\times\mathcal{R}(\xi)\big) + \sum_{\zeta\xi\in\chi_{2,2}} \big(\mathcal{R}(\zeta)\times\mathcal{R}(\xi)\big) + \sum_{\zeta\xi\in\chi_{1,2}} \big(\mathcal{R}(\zeta)\times\mathcal{R}(\xi)\big)$
$+ \sum_{\zeta\xi\in\chi_{1,2}} \big(\mathcal{R}(\zeta)\times\mathcal{R}(\xi)\big)$

$= 2(20 \times 2^{n+1} - 14) + 4(16 \times 2^{n+1} - 8) + 1(2^{n+1} - 3) + 3(6 \times 2^{n+1} - 7)$
$= 62 \times 2^{n+2} - 84$

Reverse Hyper Zagreb Index

$$\mathcal{R}HM(\delta) = \sum_{\zeta\xi \in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} (\mathcal{R}(\zeta) + \mathcal{R}(\xi))^2$$

$= \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta) + \mathcal{R}(\xi))^2 + \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta) + \mathcal{R}(\xi))^2 + \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta) + \mathcal{R}(\xi))^2$
$+ \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta) + \mathcal{R}(\xi))^2$
$= 9(20 \times 2^{n+1} - 14) + 16(16 \times 2^{n+1} - 8) + 4(2^{n+1} - 3) + 16(6 \times 2^{n+1} - 7)$
$= 270 \times 2^{n+2} - 378$

Reverse Forgotten Index

$$\mathcal{R}F(\delta) = \sum_{\zeta\xi \in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} (\mathcal{R}(\zeta)^2 + \mathcal{R}(\xi)^2)$$

$= \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta)^2 + \mathcal{R}(\xi)^2) + \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta)^2 + \mathcal{R}(\xi)^2) + \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta)^2 + \mathcal{R}(\xi)^2)$
$+ \sum_{\zeta\xi \in \chi_{1,2}} (\mathcal{R}(\zeta)^2 + \mathcal{R}(\xi)^2)$
$= 5(20 \times 2^{n+1} - 14) + 8(16 \times 2^{n+1} - 8) + 2(2^{n+1} - 3) + 10(6 \times 2^{n+1} - 7)$
$= 146 \times 2^{n+2} - 210$

Reverse Augmented Zagreb Index

$$\mathcal{R}AZI(\delta) = \sum_{\zeta\xi \in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi) - 2}\right)^3$$

$= \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi) - 2}\right)^3 + \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi) - 2}\right)^3 + \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi) - 2}\right)^3$
$+ \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi) - 2}\right)^3$
$= 8(20 \times 2^{n+1} - 14) + 8(16 \times 2^{n+1} - 8) + \left(\frac{3}{2}\right)^3 (6 \times 2^{n+1} - 7)$
$= \frac{1233 \times 2^{n+2}}{8} - \frac{1597}{8}$

Reverse First Redefined Zagreb Index

$$\mathcal{R}ReZG_1(\delta) = \sum_{\zeta\xi \in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\frac{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}\right)$$

$= \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}\right) + \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}\right) + \sum_{\zeta\xi \in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}\right)$

$+ \ \sum_{\zeta\xi\in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta)+\mathcal{R}(\xi)}{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}\right)$

$= \left(\frac{3}{2}\right)(20 \times 2^{n+1} - 14) + (16 \times 2^{n+1} - 8) + 2(2^{n+1} - 3) + \left(\frac{4}{3}\right)(6 \times 2^{n+1} - 7)$

$= 29 \times 2^{n+2} - \frac{133}{3}$

Reverse Second Redefined Zagreb Index

$$\mathcal{R}\mathrm{ReZG}_2(\delta) = \sum_{\zeta\xi\in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \left(\frac{\mathcal{R}(\zeta) \times \mathcal{R}(\xi)}{\mathcal{R}(\zeta) + \mathcal{R}(\xi)}\right)$$

$= \sum_{\zeta\xi\in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}{\mathcal{R}(\zeta)+\mathcal{R}(\xi)}\right) + \sum_{\zeta\xi\in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}{\mathcal{R}(\zeta)+\mathcal{R}(\xi)}\right) + \sum_{\zeta\xi\in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}{\mathcal{R}(\zeta)+\mathcal{R}(\xi)}\right)$
$+ \ \sum_{\zeta\xi\in \chi_{1,2}} \left(\frac{\mathcal{R}(\zeta)\times\mathcal{R}(\xi)}{\mathcal{R}(\zeta)+\mathcal{R}(\xi)}\right)$

$= \left(\frac{2}{3}\right)(20 \times 2^{n+1} - 14) + (16 \times 2^{n+1} - 8) + \left(\frac{1}{2}\right)(2^{n+1} - 3) + \left(\frac{3}{2}\right)(6 \times 2^{n+1} - 7)$

$= \frac{209\times2^{n+2}}{12} - \frac{289}{12}$

Reverse Third Redefined Zagreb Index

$$\mathcal{R}\mathrm{ReZG}_2(\delta) = \sum_{\zeta\xi\in \chi_{\mathcal{R}(\zeta),\mathcal{R}(\xi)}} \big(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\big)\big(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\big)$$

$= \sum_{\zeta\xi\in \chi_{1,2}}\big(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\big)\big(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\big) + \sum_{\zeta\xi\in \chi_{1,2}}\big(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\big)\big(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\big) +$
$\sum_{\zeta\xi\in \chi_{1,2}}\big(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\big)\big(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\big) + \sum_{\zeta\xi\in \chi_{1,2}}\big(\mathcal{R}(\zeta) + \mathcal{R}(\xi)\big)\big(\mathcal{R}(\zeta) \times \mathcal{R}(\xi)\big)$

$= 6(20 \times 2^{n+1} - 14) + 16(16 \times 2^{n+1} - 8) + 2(2^{n+1} - 3) + 12(6 \times 2^{n+1} - 7)$

$= 146 \times 2^{n+2} - 210$

4 Numerical And Graphical Comparsion

In this section, all indices whose analytical expressions are determined are given numerically. Refer to Table 4 for the same. The graphical comparison among reverse randic index, reverse atom bond connectivity index, reverse geometric index, reverse first and second Zagreb indices, reverse hyper Zagreb index, reverse forgotten index, reverse first, second and third redefined Zagreb indices and reverse augmented Zagreb index helps to predict the molecular structure and examine its properties. Refer to Figure 3 and 4 for the same. MATLAB has been used to plot the topological indices.

Indices	n=1	n=2	n=3	n=4	n=5
$\mathcal{R}R_{\frac{1}{2}}(\delta)$	239.78296	530.4893	1111.9019	2274.7271	4600.3775
$\mathcal{R}R_{\frac{1}{2}}(\delta)$	89.484	199.9086	420.7588	862.4586	1745.8582
$\mathcal{R}R_1(\delta)$	412	908	1900	3884	7852
$\mathcal{R}R_{-1}(\delta)$	57.6667	129.6667	273.6667	561.6667	1137.6667
$\mathcal{R}ReZG_1(\delta)$	187.6667	419.6667	883.6667	1711.6666	3667.6667
$\mathcal{R}ReZG_2(\delta)$	115.25	254.58333	533.25	1090.58333	2205.25
$\mathcal{R}ReZG_3(\delta)$	1506	3314	6930	14162	28626

Table 4: Numerical value of $\mathcal{R}R_{\frac{1}{2}}(\delta)$, $\mathcal{R}R_{\frac{1}{2}}(\delta)$, $\mathcal{R}R_1(\delta)$, $\mathcal{R}R_{-1}(\delta)$, $\mathcal{R}ReZG_1(\delta)$, $\mathcal{R}ReZG_2(\delta)$ and $\mathcal{R}ReZG_3(\delta)$

Indices	n=1	n=2	n=3	n=4	n=5
$\mathcal{R}ABC(\delta)$	100.1475	221.5668	464.4054	950.0825	1921.4369
$\mathcal{R}RGA(\delta)$	137.9478	306.1572	642.5758	1315.4132	2661.0878
$\mathcal{R}M_1(\delta)$	500	1108	2324	4756	9620
$\mathcal{R}M_2(\delta)$	412	908	1900	3884	7852
$\mathcal{R}HM(\delta)$	1782	3942	8262	16902	34182
$\mathcal{R}F(\delta)$	958	2126	4462	9134	18478
$\mathcal{R}AZI(\delta)$	1033.375	2266.375	4732.375	9664.375	19528.375

Table 5: Numerical value of $\mathcal{R}ABC(\delta)$, $\mathcal{R}RGA(\delta)$, $\mathcal{R}M_1(\delta)$, $\mathcal{R}M_2(\delta)$, $\mathcal{R}HM(\delta)$, $\mathcal{R}F(\delta)$ and $\mathcal{R}AZI(\delta)$

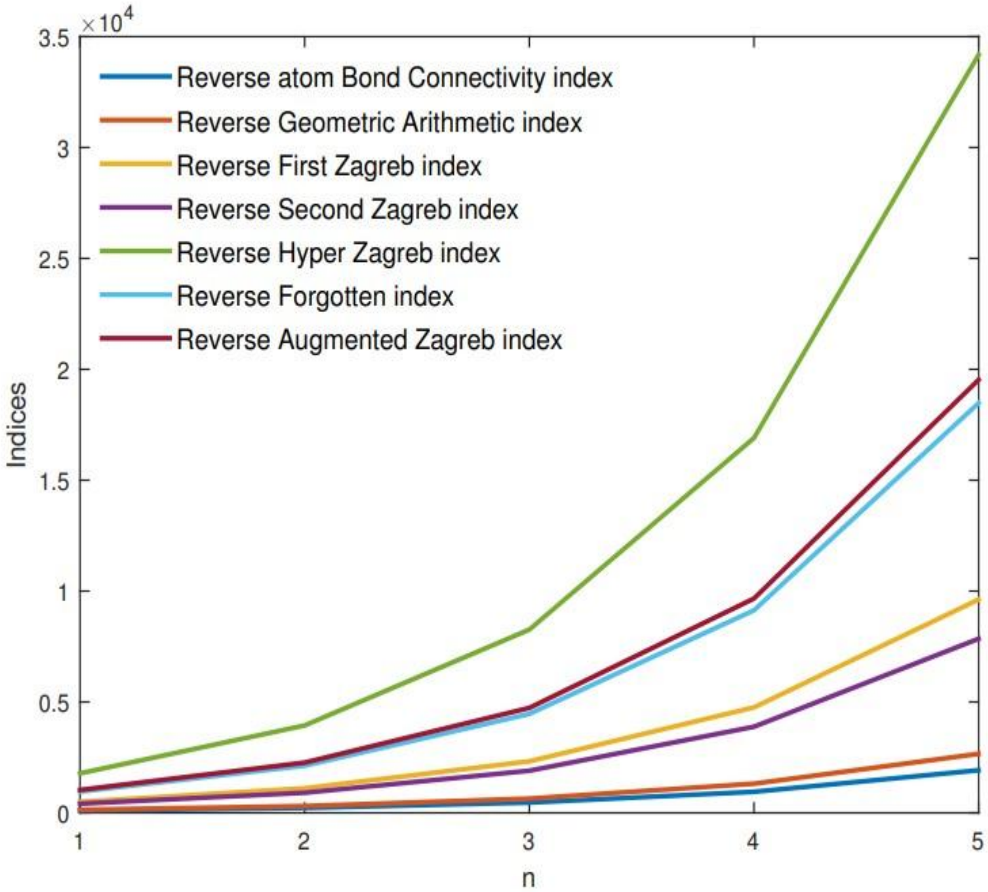

Figure 3: Graphical comparison of $\mathcal{R}ABC(\delta)$, $\mathcal{R}RGA(\delta)$, $\mathcal{R}M_1(\delta)$, $\mathcal{R}M_2(\delta)$, $\mathcal{R}HM(\delta)$, $\mathcal{R}F(\delta)$ and $\mathcal{R}AZI(\delta)$ for CD_n.

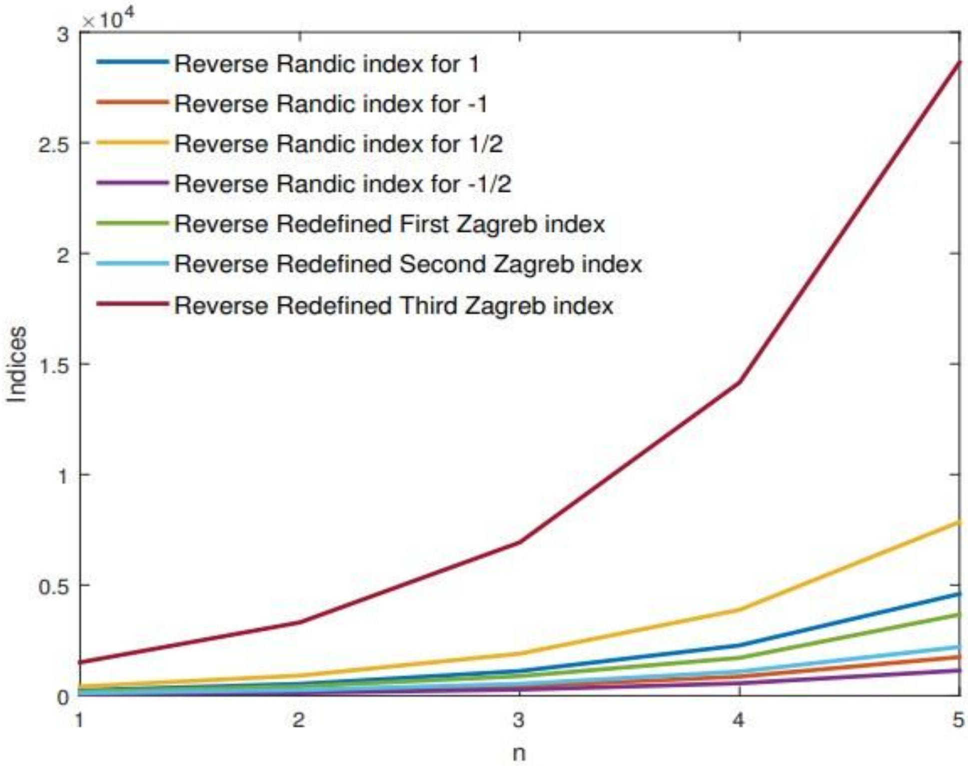

Figure 4: Graphical comparison of $\mathcal{R}\mathrm{R}_{\frac{1}{2}}(\delta)$, $\mathcal{R}\mathrm{R}_{\frac{1}{2}}(\delta)$, $\mathcal{R}\mathrm{R}_{1}(\delta)$, $\mathcal{R}\mathrm{R}_{-1}(\delta)$, $\mathcal{R}\mathrm{ReZG}_{1}(\delta)$, $\mathcal{R}\mathrm{ReZG}_{2}(\delta)$ and $\mathcal{R}\mathrm{ReZG}_{3}(\delta)$ for CD_{n}

4. Conclusion

In this article, reverse degree-based topological descriptors namely reverse randic index, reverse redefined Zagreb indices, reverse Zagreb indices, reverse forgotten index, reverse geometric arithmetic index and reverse atom bond connectivity index for chiral PAMAM dendrimer, CD_{n} have been evaluated. It is possible that the computed results could gain a deeper understanding of the nature and behaviour of Chiral PAMAM dendrimer. The graphical representation of the numerical values identifies indices with similar behaviours.

5. References

Kowalski, P. S., Rudra, A., Miao, L., & Anderson, D. G. (2019). Delivering the messenger: advances in technologies for therapeutic mRNA delivery. Molecular Therapy, 27(4), 710-728.

García, I., Fall, Y., & Gómez, G. (2010). Using topological indices to predict anti-Alzheimer and anti-parasitic GSK-3 inhibitors by multi-target QSAR in silico screening. Molecules, 15(8), 5408-5422.

Cioslowski, J. (1985). Additive nodal increments for approximate calculation of the total π-electron energy of benzenoid hydrocarbons. Theoretica chimica acta, 68, 315-319.

Hu, M., Ali, H., Binyamin, M. A., Ali, B., Liu, J. B., & Fan, C. (2021). On distance-based topological descriptors of chemical interconnection networks. Journal of Mathematics, 2021, 1-10.

Xavier, D. A., Akhila, S., Alsinai, A., Julietraja, K., Ahmed, H., Raja, A. A., & Varghese, E. S. (2022). Distance-Based Structure Characterization of PAMAM-Related

Dendrimers Nanoparticle. Journal of Nanomaterials, 2022.

Pittelkow, M., Brock-Nannestad, T., Moth-Poulsen, K., & Christensen, J. B. (2008). Chiral dendrimer encapsulated Pd and Rh nanoparticles. Chemical communications, (20), 2358-2360.

Wei, J., Cancan, M., Rehman, A. U., Siddiqui, M. K., Nasir, M., Younas, M. T., & Hanif, M. F. (2022). On topological indices of remdesivir compound used in treatment of Corona virus (COVID 19). Polycyclic Aromatic Compounds, 42(7), 4300-4316.

Zhao, D., Chu, Y. M., Siddiqui, M. K., Ali, K., Nasir, M., Younas, M. T., & Cancan, M. (2022). On reverse degree based topological indices of polycyclic metal organic network. Polycyclic Aromatic Compounds, 42(7), 4386-4403.

Poojary, P., Shenoy, G. B., Swamy, N. N., Ananthapadmanabha, R., Sooryanarayana, B., & Poojary, N. (2022). Reverse topological indices of some molecules in drugs used in the treatment of h1n1. Biointerface Res. Appl. Chem., 13(1), 71.

Ravi, V., & Desikan, K. (2023). Curvilinear regression analysis of benzenoid hydrocarbons and computation of some reduced reverse degree based topological indices for hyaluronic acid-paclitaxel conjugates. Scientific Reports, 13(1), 3239.

Kulli, V. R. (2018). Reverse Zagreb and reverse hyper-Zagreb indices and their polynomials of rhombus silicate networks. Annals of Pure and Applied Mathematics, 16(1), 47-51.

Randic, M. (1975). Characterization of molecular branching. Journal of the American Chemical Society, 97(23), 6609-6615.

Estrada, E., Torres, L., Rodriguez, L., & Gutman, I. (1998). An atom-bond connectivity index: modelling the enthalpy of formation of alkanes.

Vukičević, D., & Furtula, B. (2009). Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. Journal of mathematical chemistry, 46, 1369-1376.

Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. Chemical physics letters, 17(4), 535-538.

Gutman, I., & Das, K. C. (2004). The first Zagreb index 30 years after. MATCH Commun. Math. Comput. Chem, 50(1), 83-92.

Shirdel, G. H., Rezapour, H., & Sayadi, A. M. (2013). The hyper-Zagreb index of graph operations.

Furtula, B., & Gutman, I. (2015). A forgotten topological index. Journal of mathematical chemistry, 53(4), 1184-1190.

Furtula, B., Graovac, A., & Vukičević, D. (2010). Augmented zagreb index. Journal of mathematical chemistry, 48, 370-380.

Ranjini, P. S., Lokesha, V., & Usha, A. (2013). Relation between phenylene and hexagonal squeeze using harmonic index. Int. J. Graph Theory, 1(4), 116-121.