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Neighborhood-Based Descriptors for Porphyrin Dendrimers

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Abstract: The symmetry of molecular structures is captured by topological indices, which provide a mathematical vocabulary for predicting features such as boiling temperatures, viscosity, and gyration radius and are also employed in QSPR/QSAR research. Dendrimers are a brand-new type of polymer. It is characterized as a macromolecule due to its highly radiated structure, providing great water solubility and adaptability. Because of these features, dendrimers are a strong alternative for medication delivery. This article investigates some topological indices based on neighborhood degrees such as Modified Randic index, Inverse Sum Index, SK, SK1, and SK2 index for some dendrimers.

Keywords: Neighborhood indices; porphyrin dendrimers; poly(propyl) ether imine dendrimer.

1. Introduction

An important use of (connected undirected) graphs is representing an atomic structure by a molecular graph where the node represents atoms, and the edges indicate bondings. This is explored in a discipline called chemical graph theory. The overall topological structure of such a network can be captured in a single number known as a chemical index or a topological index [1-3], which is frequently linked to chemical attributes.

G(V,E) is a graph in which V denotes the set of vertices and E denotes the set of edges linking the vertices. The degree of a vertex v in graph G is the number of edges incident with v, symbolized by deg(v). A graph in which each pair of vertices is connected is known as a connected graph. The set of all vertices adjacent to u is denoted by N(u) and defined as a Neighborhood set of u. The sum degree of vertex u is defined as $S(u) = \sum_{v \in N(u)} \deg(v)$[4].

Dendrimers are branching polymeric molecules with a high degree of organization. Dendrimers are symmetric about the core, which have a spherical 3D topology. A core, an inner, and an outer shell are the three major components of dendrimers. To regulate features such as solubility, thermal stability, and chemical attachment for different tasks, a dendrimer can be synthesized with varied functionality in each of these components. It has an ancient legacy of use in targeted, ophthalmic, pulmonary, transdermal, and gene-drug delivery [5-10]. Since it is difficult to synthesize dendrimers, they are difficult to produce and expensive to buy. Analyzing topological indices for dendrimers is an effective way to eliminate the cost and time-consuming laboratory research.

Numerous studies[11-32] have described and determined topological indices of dendrimers like Poly propyl ether imine dendrimer, porphyrin dendrimers, Poly EThylene

Amido Amine Dendrimer, Phosphorus-Containing Dendrimers, PDI-Cored Dendrimers, Triazine-Based Dendrimers, and Aliphatic Polyamide Dendrimers.

Several research [33-40] have begun to look into Neighborhood-based topological indices. Vignesh Ravi and Kalyani Desikan proposed some Neighborhood-based descriptors, namely SK_N, $SK1_N$, $SK2_N$, Modified Randić index(mR_N), and Inverse Sum Index(ISI_N)[33]. The indices are given below in equations (1) to (5).

$$SK_N(G)=\sum_{uv\in E}\left[\frac{S(u)+S(v)}{2}\right] \quad (1)$$

$$SK1_N(G)=\sum_{uv\in E}\left[\frac{S(u)\ \mathrm{x}\ S(v)}{2}\right] \quad (2)$$

$$SK2_N(G)=\sum_{uv\in E}\left(\frac{S(u)+S(v)}{2}\right)^2 \quad (3)$$

$$mR_N(G)=\sum_{uv\in E}\left(\frac{1}{\max\{S(u),S(v)\}}\right) \quad (4)$$

$$ISI_N(G)=\sum_{uv\in E}\left(\frac{S(u)\mathrm{x}\,S(v)}{S(u)+S(v)}\right) \quad (5)$$

In this paper, we evaluate the above-mentioned indices for Poly propyl ether imine (PETIM) dendrimer, Zinc porphyrin (DPZ_g) dendrimer, and Porphyrin (D_gP_g) dendrimer. We also use MATLAB to depict the 2D representations of the indices.

2. Materials and Methods

The Neighborhood degree-based topological indices of dendrimers are our most important computational results. The results were analyzed using the edge partition method and graph-theoretical ideas. In Figures 5–14, the outcomes are visually depicted using MATLAB R2020a.

3. Results and Discussion

3.1. PETIM dendrimer.

The polynomial of PETIM dendrimer expands from the oxygen as the base and sprouts out at each tertiary nitrogen, which is separated by an eight-bond spacer in every iteration of the dendrimer. Figure 1 shows g growth stages for the molecular graph G of PETIM dendrimer with generation G_g. The PETIM dendrimer graph is composed of four wings and an eight-edged central core. In each branch, we have$8 + 2 \mathrm{x} 8 + 2^2\mathrm{x} 8 + \ldots + 2^{g-2}\mathrm{x} 8 + 4 \mathrm{x} 2^{g-1} = 6 \mathrm{x} 2^g– 8$ edges. Also, the total number of bonds in G is$(24 \mathrm{x} 2^g) – 24$. By this, the number of atoms in G can be given directly as $(24 \mathrm{x} 2^g) – 23$ since it is a tree [11].

The total number of vertices with degree 1 in G_g is 2^{g+1}, which is the number of leaves in the tree. The vertices of degree 3 and degree 2 are $2^{g+1}– 2$ and $20 \mathrm{x} 2^g– 21$, respectively.For the pair (S(u),S(v)) where uv∈E(G) the edges are partitioned as $2 \mathrm{x} 2^g$ for the pairs (2,3) and (3,4); $8 \mathrm{x} 2^g– 12$ for the pair (4,4) and $6 \mathrm{x} 2^g – 6$ for the pairs (4,5) and (5,6).

3.1.1. Theorem: SK_N (PETIM) = $104 \times 2^g - 108$.

Proof:

SK_N (PETIM)$=\sum_{uv\in E}\frac{S(u)+S(v)}{2}$

$= 2 \mathrm{x} 2^g\left(\frac{2+3}{2}\right)+ 2 \mathrm{x} 2^g\left(\frac{3+4}{2}\right) + (8 \mathrm{x} 2^g– 12)\left(\frac{4+4}{2}\right) + (6 \mathrm{x} 2^g– 6)\left(\frac{4+5}{2}\right) + (6 \mathrm{x} 2^g– 6)\left(\frac{5+6}{2}\right)$

$= (5 \mathrm{x} 2^g) + (7 \mathrm{x} 2^g) + 4(8 \mathrm{x} 2^g -12) + (9 \mathrm{x} 3)(2^g- 1) + (11 \mathrm{x} 3)(2^g- 1)$

$= 104 \times 2^g - 108.$

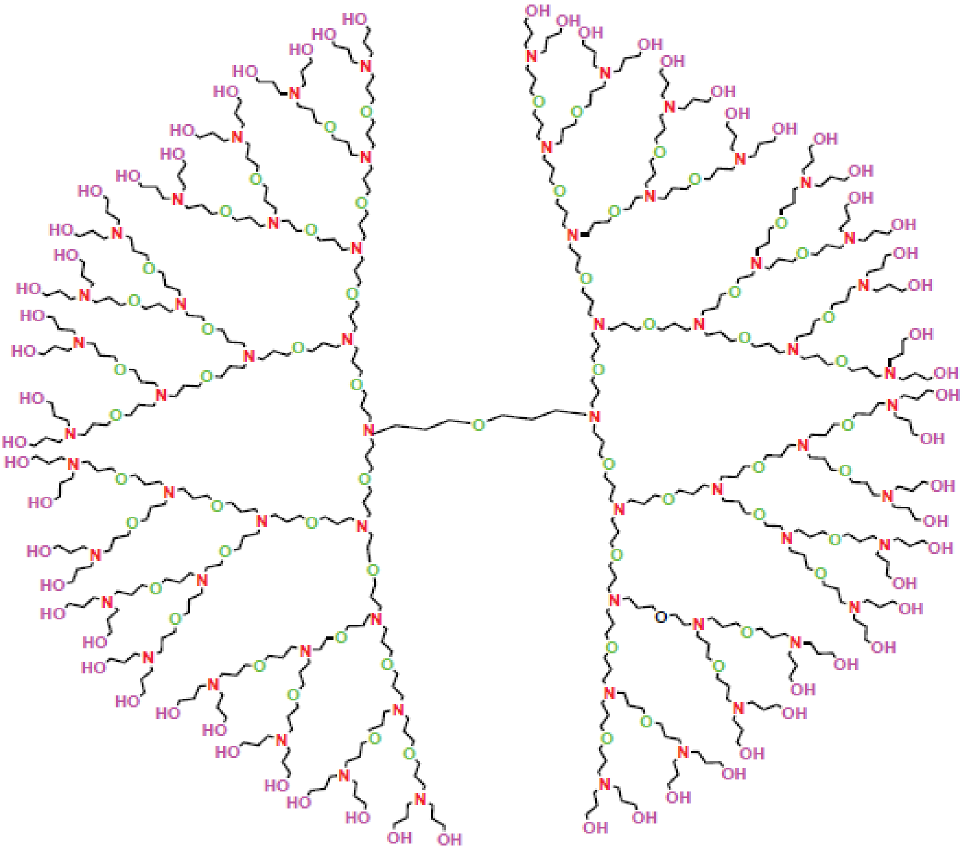


Figure 1. PETIM dendrimer molecular structure.

3.1.2. Theorem $SK1_N$ (PETIM) $= 232 \times 2^g - 246$.

Proof:

$SK1_N$ (PETIM)$=\sum_{uv \in E} \frac{S(u) \times S(v)}{2}$

$= 2 \times 2^g\left(\frac{2 \times 3}{2}\right) + 2 \times 2^g\left(\frac{3 \times 4}{2}\right) + (8 \times 2^g - 12)\left(\frac{4 \times 4}{2}\right) + (6 \times 2^g - 6)\left(\frac{4 \times 5}{2}\right)$

$+ (6 \times 2^g - 6)\left(\frac{5 \times 6}{2}\right)$

$= (2 \times 2^g \times 3) + (2 \times 2^g \times 6) + 8(8 \times 2^g - 12) + 10(6 \times 2^g - 6) + 15(6 \times 2^g - 6)$

$= 232 \times 2^g - 246.$

3.1.3. Theorem $SK2_N$ (PETIM) $= 468 \times 2^g - 495$.

Proof:

SK2N (PETIM)$=\sum_{uv \in E} \left(\frac{S(u)+S(v)}{2}\right)^2$

$= 2 \times 2^g\left(\frac{2+3}{2}\right)^2 + 2 \times 2^g\left(\frac{3+4}{2}\right)^2 + (8 \times 2^g - 12)\left(\frac{4+4}{2}\right)^2 + (6 \times 2^g - 6)\left(\frac{4+5}{2}\right)^2$

$+ (6 \times 2^g - 6)\left(\frac{5+6}{2}\right)^2$

$= \left(\frac{25}{2} \times 2^g\right) + \left(\frac{49}{2} \times 2^g\right) + \frac{64}{2}(4 \times 2^g - 6) + \frac{81}{2}(3 \times 2^g - 3) + \frac{121}{2}(3 \times 2^g - 3)$

$= 468 \times 2^g - 495.$

3.1.4. Theorem: mR_N (PETIM) $= \frac{161}{30} \times 2^g - \frac{26}{5}$.

Proof:

mR_N (PETIM)=$\sum_{uv\in E}\left(\frac{1}{\max\{S(u),S(v)\}}\right)$

$= (2 \text{ x } 2^g)\left(\frac{1}{\max\{2,3\}}\right) + (2 \text{ x } 2^g)\left(\frac{1}{\max\{3,4\}}\right) + (8 \text{ x } 2^g - 12)\left(\frac{1}{\max\{4,4\}}\right)$

$+ (6 \text{ x } 2^g - 6)\left(\frac{1}{\max\{4,5\}}\right) + (6 \text{ x } 2^g - 6)\left(\frac{1}{\max\{5,6\}}\right)$

$= (2 \text{ x } 2^g \text{x } \frac{1}{3}) + (2 \text{ x } 2^g \text{x } \frac{1}{4}) + \frac{1}{4}(8 \text{ x } 2^g - 12) + \frac{1}{5}(6 \text{ x} 2^g - 6) + \frac{1}{6}(6 \text{ x } 2^g - 6)$

$= \frac{161}{30} \times 2^g - \frac{26}{5}$.

3.1.5. Theorem ISI_N (PETIM) = $\frac{59512}{1155} \times 2^g - \frac{14176}{264}$.

Proof:

ISI_N (PETIM)=$\sum_{uv\in E}\left(\frac{S(u) \text{x } S(v)}{S(u)+S(v)}\right)$

$=(2 \text{ x } 2^g)\left(\frac{2 \text{ x } 3}{2+3}\right) + (2 \text{ x } 2^g)\left(\frac{3 \text{ x } 4}{3+4}\right) + (8 \text{ x } 2^g - 12)\left(\frac{4 \text{ x } 4}{4+4}\right) + (6 \text{ x } 2^g - 6)\left(\frac{4 \text{ x } 5}{4+5}\right)$

$+ (6 \text{ x } 2^g - 6)\left(\frac{5 \text{ x } 6}{5+6}\right)$

$= (2 \text{ x } 2^g \text{x } \frac{6}{5}) + (2 \text{ x } 2^g \text{x } \frac{12}{7}) + \frac{16}{8}(8 \text{ x } 2^g - 12) + \frac{20}{9}(6 \text{ x} 2^g - 6) + \frac{30}{11}(6 \text{ x } 2^g - 6)$

$= \frac{59512}{1155} \times 2^g - \frac{14176}{264}$.

3.2. DPZ_g dendrimer.

DPZ_g has four identical branches and a central core in its molecular graph. DPZ_g has 96g-10 atoms and 105g-11 bonds in its molecular graph. The edge-set partition of DPZ_g are shown [11]as 8 x 2^g for the pair (4,4), 8 for the pairs (4,5), (5,8), (8,9) and (8.10), 16 x 2^g– 12 for the pairs (5,5) and (5,7), 8 x 2^g – 12 for the pair (5,6), 8 x 2^g – 12 for the pair (7,8) , 4 x 2^g for the pair (6,6), 4 for the pairs (6,7), (7,9) and (10,12), 4 x 2^g – 4 for the pair (6,8).Figure 2 depicts the chemical structure of the zinc porphyrin dendrimer DPZ_g.

Theorem 3.2.1: SK_N (DPZ_g) = 324 × 2^g + 44.

Proof:

SK_N (DPZ_g)= $(8 \text{ x } 2^g)\left(\frac{4+4}{2}\right) + 8\left(\frac{4+5}{2}\right) + (16 \text{ x } 2^g - 12)\left(\frac{5+5}{2}\right) + (8 \text{ x } 2^g - 12)\left(\frac{5+6}{2}\right)$

$+ (16 \text{ x } 2^g - 12)\left(\frac{5+7}{2}\right) + 8\left(\frac{5+8}{2}\right) + (4 \text{ x } 2^g)\left(\frac{6+6}{2}\right) + 4\left(\frac{6+7}{2}\right) + (4 \text{ x } 2^g - 4)\left(\frac{6+8}{2}\right)$

$+ (8 \text{ x } 2^g - 8)\left(\frac{7+8}{2}\right) + 4\left(\frac{7+9}{2}\right) + 8\left(\frac{8+9}{2}\right) + 8\left(\frac{8+10}{2}\right) + 4\left(\frac{10+12}{2}\right)$

$= (32 \text{ x } 2^g) + 36 + (80 \text{ x } 2^g) - 60 + (4 \text{ x } 2^g) - 66 + (96 \text{ x} 2^g) - 72 + 52 + (24 \text{ x } 2^g) + 26$

$+ (28 \text{ x } 2^g) - 28 + (60 \text{ x } 2^g) - 60 + 32 + 68 + 72 + 44$

$= 324 \times 2^g + 44$.

3.2.2. Theorem $SK1_N$ (DPZ_g) = 1056 × 2^g + 438.

Proof:

$SK1_N$ (DPZ_g)= $(8 \text{ x } 2^g)\left(\frac{4 \text{ x } 4}{2}\right) + 8\left(\frac{5 \text{ x } 4}{2}\right) + (16 \text{ x } 2^g - 12)\left(\frac{5 \text{ x } 5}{2}\right) + (8 \text{ x } 2^g - 12)\left(\frac{5 \text{ x } 6}{2}\right)$

$+ (16 \text{ x } 2^g - 12)\left(\frac{5 \text{ x } 7}{2}\right) + 8\left(\frac{5 \text{ x } 8}{2}\right) + (4 \text{ x } 2^g)\left(\frac{6 \text{ x } 6}{2}\right) + 4\left(\frac{6 \text{ x } 7}{2}\right) + (4 \text{ x } 2^g - 4)\left(\frac{6 \text{ x } 8}{2}\right)$

$+ \ (8 \text{ x } 2^g\text{- } 8)\left(\frac{7 \text{ x } 8}{2}\right) + 4\left(\frac{7 \text{ x } 9}{2}\right) + \ 8\left(\frac{8 \text{ x } 9}{2}\right) + \ 8\left(\frac{8 \text{ x } 10}{2}\right) + \ 4\left(\frac{10 \text{ x } 12}{2}\right)$

$= (8 \text{ x } 2^g\text{x } 8) + 80 + \frac{25}{2}(16 \text{ x } 2^g\text{- } 12) + 15(8 \text{ x } 2^g \text{ -}12) + \frac{35}{2}(16 \text{ x} 2^g\text{- } 12) + 160 + (18 \text{ x } 4 \text{ x } 2^g)$

$+ 84 + 24(4 \text{ x } 2^g \text{ - } 4) + 28(8 \text{ x } 2^g \text{ - } 8) + 126 + 288 + 320 + 240$

$= 1056 \times 2^g + 438.$

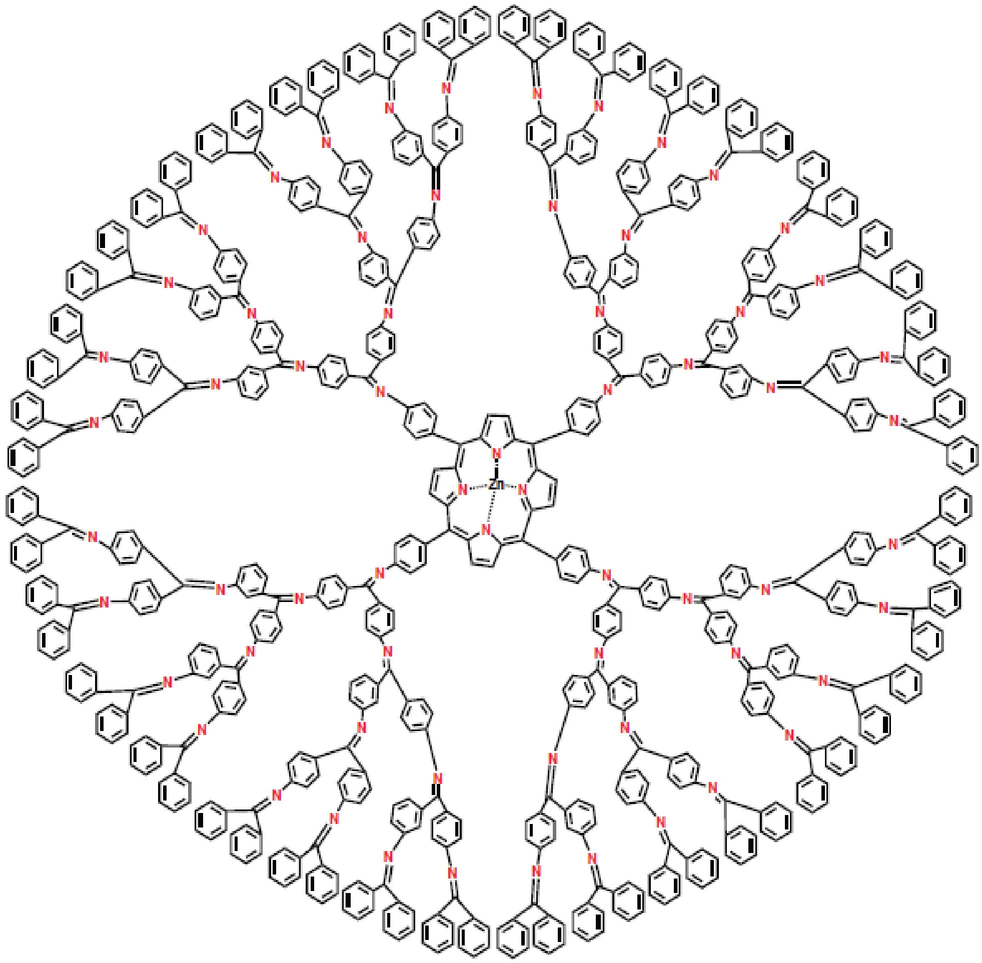


Figure 2. Zinc porphyrin dendrimer DPZ_gmolecular structure.

3.2.3. Theorem $SK2_N$ (DPZ_g) = $2136 \times 2^g + 894$.

Proof:

$SK2_N\ (DPZ_g)= (8 \text{ x } 2^g)\ \left(\frac{4+4}{2}\right)^2 + 8\left(\frac{5+4}{2}\right)^2 + (16 \text{ x } 2^g-12)\left(\frac{5+5}{2}\right)^2 + (8 \text{ x } 2^g- 12)\left(\frac{5+6}{2}\right)^2$

$+ (16 \text{ x } 2^g- 12)\left(\frac{5+7}{2}\right)^2 + 8\left(\frac{5+8}{2}\right)^2 + (4 \text{ x } 2^g)\left(\frac{6+6}{2}\right)^2 + 4\left(\frac{6+7}{2}\right)^2 + (4 \text{ x } 2^g- 4)\left(\frac{6+8}{2}\right)^2$

$+ (8 \text{ x } 2^g-8)\left(\frac{7+8}{2}\right)^2 + 4\left(\frac{7+9}{2}\right)^2 + 8\left(\frac{8+9}{2}\right)^2 + 8\left(\frac{8+10}{2}\right)^2 + 4\left(\frac{10+12}{2}\right)^2$

$= (8 \text{ x } 16 \text{ x } 2^g) + (2 \text{ x } 81) +(16 \text{ x } 25 \text{ x } 2^g) \text{ - } (12 \text{ x } 25) + (121 \text{ x } 2 \text{ x } 2^g) - (121 \text{ x } 3)$

$+ (36 \text{ x } 16 \text{ x } 2^g) - (36 \text{ x } 12) + (2 \text{ x } 169) + (36l \text{ x } 4 \text{ x } 2^g) + 169 + (49 \text{ x } 4 \text{ x } 2^g)$

$- (49 \text{ x } 4) + (225 \text{ x } 2 \text{ x } 2^g) - (225 \text{ x } 2) + (4 \text{ x } 64) + (2 \text{ x } 289) + (8 \text{ x } 81) + 484$

$= 2136 \times 2^g + 894.$

3.2.4. Theorem mR_N (DPZ_g) = $\frac{2307}{210} \times 2^g - \frac{41}{42}$.

Proof:

mR_N (DPZ_g)= $(8 \times 2^g)\left(\frac{1}{\max\{4,4\}}\right)+ 8\left(\frac{1}{\max\{5,4\}}\right) + (16 \times 2^g - 12)\left(\frac{1}{\max\{5,5\}}\right)$
$+ (8 \times 2^g - 12)\left(\frac{1}{\max\{5,6\}}\right) + (16 \times 2^g - 12)\left(\frac{1}{\max\{5,7\}}\right) + 8\left(\frac{1}{\max\{5,8\}}\right) + (4 \times 2^g)\left(\frac{1}{\max\{6,6\}}\right)$
$+ 4\left(\frac{1}{\max\{6,7\}}\right)+ (4 \times 2^g - 4)\left(\frac{1}{\max\{6,8\}}\right) + (8 \times 2^g - 8)\left(\frac{1}{\max\{7,8\}}\right) + 4\left(\frac{1}{\max\{7,9\}}\right)$
$+ 8\left(\frac{1}{\max\{8,9\}}\right) + 8\left(\frac{1}{\max\{8,10\}}\right) + 4\left(\frac{1}{\max\{10,12\}}\right)$
$= \frac{1}{4}(8 \times 2^g)+ 8\left(\frac{1}{5}\right) + \frac{1}{5}(16 \times 2^g - 12) + \frac{1}{6}(8 \times 2^g - 12)+ \frac{1}{7}(16 \times 2^g - 12)+ 8\left(\frac{1}{8}\right)$
$+ \frac{1}{6}(4 \times 2^g)+ 4\left(\frac{1}{7}\right) + \frac{1}{8}(4 \times 2^g - 4)+ \frac{1}{8}(8 \times 2^g - 8)+4\left(\frac{1}{9}\right) + 8\left(\frac{1}{9}\right) + 8\left(\frac{1}{10}\right) + 4\left(\frac{1}{12}\right)$
$= \frac{2307}{210} \times 2^g - \frac{41}{42}$.

3.2.5. Theorem ISI_N (DPZ_g) = $\frac{215522}{1155} \times 2^g - \frac{64367463}{3063060}$.

Proof:
ISI_N (DPZ_g)= $(8 \times 2^g)\left(\frac{4 \times 4}{4+4}\right)+ 8\left(\frac{5 \times 4}{5+4}\right) + (16 \times 2^g - 12)\left(\frac{5 \times 5}{5+5}\right) + (8 \times 2^g - 12)\left(\frac{5 \times 6}{5+6}\right)$
$+ (16 \times 2^g - 12)\left(\frac{5 \times 7}{5+7}\right) + 8\left(\frac{5 \times 8}{5+8}\right) + (4 \times 2^g)\left(\frac{6 \times 6}{6+6}\right) + 4\left(\frac{6 \times 7}{6+7}\right) + (4 \times 2^g - 4)\left(\frac{6 \times 8}{6+8}\right)$
$+ (8 \times 2^g - 8)\left(\frac{7 \times 8}{7+8}\right) +4\left(\frac{7 \times 9}{7+9}\right) + 8\left(\frac{8 \times 9}{8+9}\right) + 8\left(\frac{8 \times 10}{8+10}\right) + 4\left(\frac{10 \times 12}{10+12}\right)$
$= \frac{215522}{1155} \times 2^g - \frac{64367463}{3063060}$.

3.3. D_gP_g dendrimer.

D_gP_g molecular graph comprises four comparable wings and a center core with five more edges (Figures 3 and 4). The total number of atoms in porphyrin dendrimer [11] is 96g–10, and the number of bonds in D_gP_g is 105g- 11. Note that $g = 2^t$, where$t \geq 2$. The edge-set partition of D_gP_g are given as 2g, g+1, 8g-6, 24g, 4g, 4g-6,6g, 18g, 25g, 11g for the pairs (3,5), (4,4), (4,5), (4,6), (5,5), (5,6), (5,7), (6,7), (6,8) and (7,9) respectively and g for the pairs (7,8) and (8,9).

3.3.1. Theorem SK_N (D_gP_g) = 642g - 56.

Proof:
SK_N (D_gP_g)= $2g\left(\frac{3+5}{2}\right)+ (g+1)\left(\frac{4+4}{2}\right) + (8g-6)\left(\frac{4+5}{2}\right) + 24g\left(\frac{4+6}{2}\right) + 4g\left(\frac{5+5}{2}\right)$
$+ (4g-6)\left(\frac{5+6}{2}\right)+ 6g\left(\frac{5+7}{2}\right)+ 18g\left(\frac{6+7}{2}\right)+ 25g\left(\frac{6+8}{2}\right)+ g\left(\frac{7+8}{2}\right) + 11g\left(\frac{7+9}{2}\right)+ g\left(\frac{8+9}{2}\right)$
= 8g + 4g + 4 + 36g – 27+120g + 20g + 22g - 33 + 36g + 117g + 175g
$+\frac{15g}{2}$ +88g $+\frac{17g}{2}$
= 642g - 56.

3.3.2. Theorem $SK1_N$ (D_gP_g) = 1994.5g - 142.

Proof:
$SK1_N$ (D_gP_g)= $2g\left(\frac{3 \times 5}{2}\right)+ (g+1)\left(\frac{4 \times 4}{2}\right) + (8g-6)\left(\frac{4 \times 5}{2}\right) + 24g\left(\frac{4 \times 6}{2}\right) + 4g\left(\frac{5 \times 5}{2}\right)$
$+ (4g-6)\left(\frac{5 \times 6}{2}\right)+ 6g\left(\frac{5 \times 7}{2}\right) + 18g\left(\frac{6 \times 7}{2}\right) + 25g\left(\frac{6 \times 8}{2}\right) + g\left(\frac{7 \times 8}{2}\right) + 11g\left(\frac{7 \times 9}{2}\right) + g\left(\frac{8 \times 9}{2}\right)$
= 15g + 8g + 8 + 80g – 60 + 288g + 50g + 60g – 90 +105g + 378g + 600g

$$+ 28g + \frac{693g}{2} + 36g$$
$$= 1994.5g -142.$$

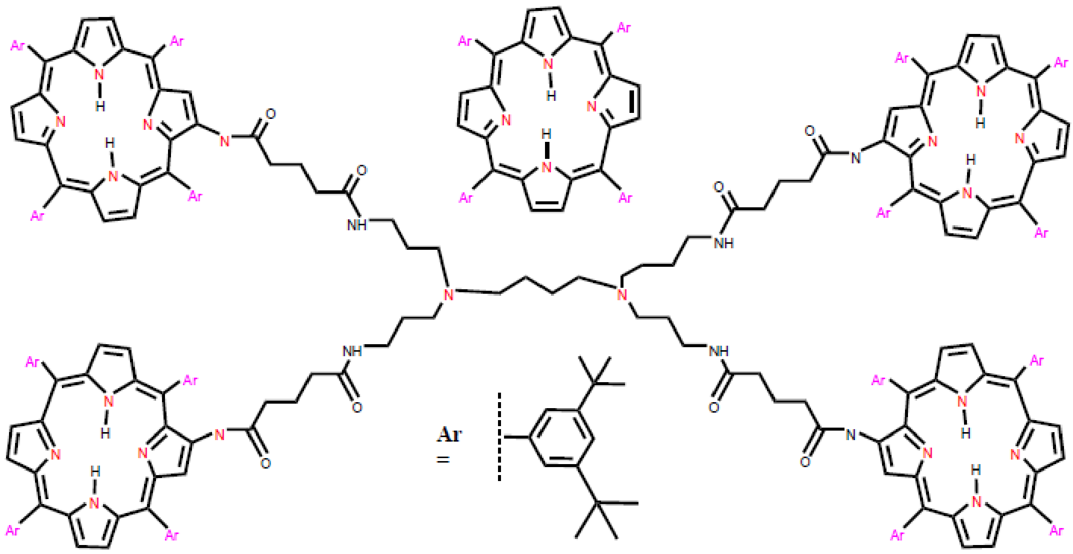


Figure 3. Porphyrin DendrimerD_4P_4molecular graph.

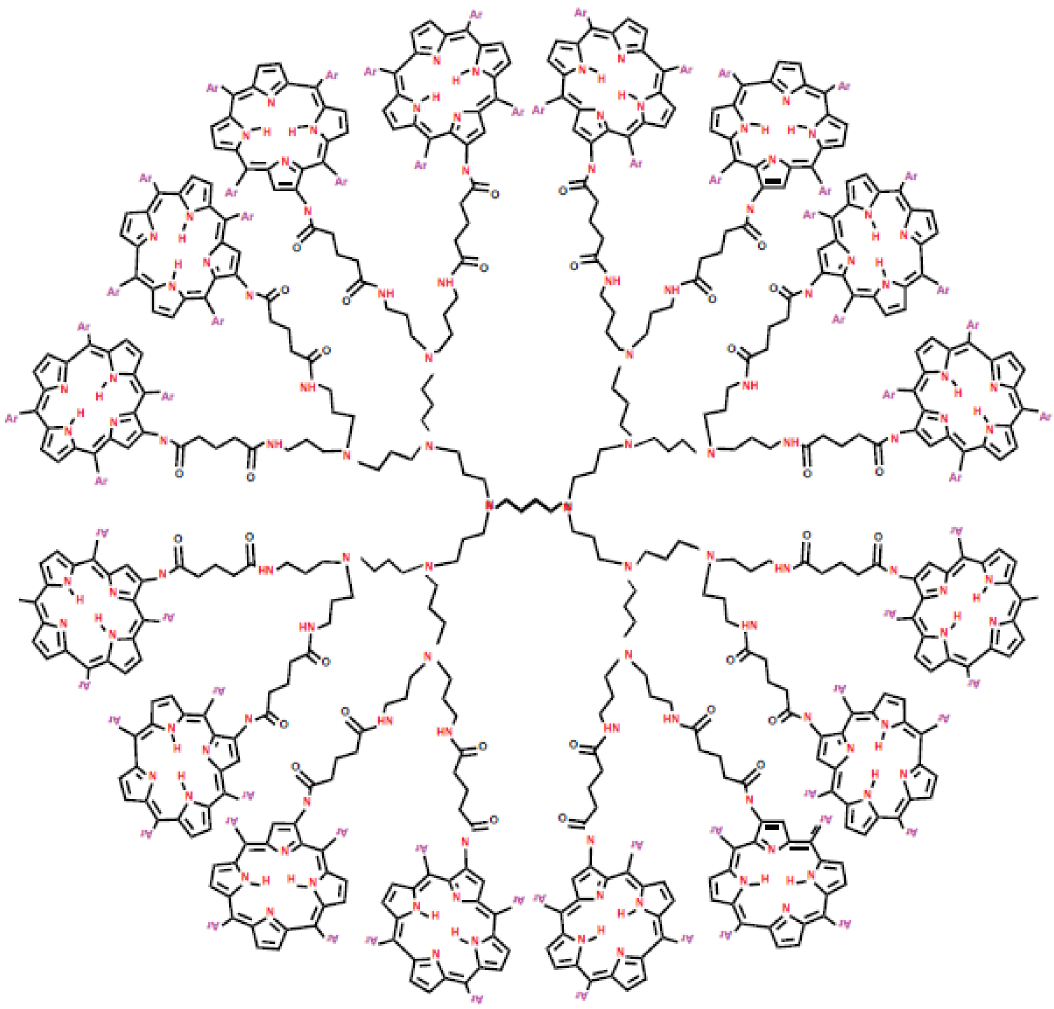


Figure 4. Porphyrin Dendrimer $D_{16}P_{16}$ molecular graph.

3.3.3. Theorem $SK2_N$ (D_gP_g) is 4065g - 287.

Proof:

$$SK2_N\,(D_gP_g) = 2g\left(\frac{3+5}{2}\right)^2 + (g+1)\left(\frac{4+4}{2}\right)^2 + (8g-6)\left(\frac{4+5}{2}\right)^2 + 24g\left(\frac{4+6}{2}\right)^2 + 4g\left(\frac{5+5}{2}\right)^2$$
$$+(4g-6)\left(\frac{5+6}{2}\right)^2 + 6g\left(\frac{5+7}{2}\right)^2 + 18g\left(\frac{6+7}{2}\right)^2 + 25g\left(\frac{6+8}{2}\right)^2 + g\left(\frac{7+8}{2}\right)^2 + 11g\left(\frac{7+9}{2}\right)^2 + g\left(\frac{8+9}{2}\right)^2$$
$$= 4065g - 287.$$

3.3.4. Theorem mR_N $(D_gP_g) = \frac{1101g}{70} - \frac{39}{20}$.

Proof:

$$mR_N\,(D_gP_g) = 2g\left(\frac{1}{\max\{3,5\}}\right) + (g+1)\left(\frac{1}{\max\{4,4\}}\right) + (8g-6)\left(\frac{1}{\max\{4,5\}}\right) + 24g\left(\frac{1}{\max\{4,6\}}\right)$$
$$+ 4g\left(\frac{1}{\max\{5,5\}}\right) + (4g-6)\left(\frac{1}{\max\{5,6\}}\right) + 6g\left(\frac{1}{\max\{5,7\}}\right) + 18g\left(\frac{1}{\max\{6,7\}}\right)$$
$$+ 25g\left(\frac{1}{\max\{6,8\}}\right) + g\left(\frac{1}{\max\{7,8\}}\right) + 11g\left(\frac{1}{\max\{7,9\}}\right) + g\left(\frac{1}{\max\{8,9\}}\right)$$
$$= 2g\left(\frac{1}{5}\right) + (g+1)\left(\frac{1}{4}\right) + (8g-6)\left(\frac{1}{5}\right) + 24g\left(\frac{1}{6}\right) + 4g\left(\frac{1}{5}\right) + (4g-6)\left(\frac{1}{6}\right) + 6g\left(\frac{1}{7}\right)$$
$$+ 18g\left(\frac{1}{7}\right) + 25g\left(\frac{1}{8}\right) + g\left(\frac{1}{8}\right) + 11g\left(\frac{1}{9}\right) + g\left(\frac{1}{9}\right)$$
$$= \frac{1101g}{70} - \frac{39}{20}.$$

3.3.5. Theorem ISI_N $(D_gP_g) = \frac{771121993g}{2450448} - \frac{914}{33}$.

Proof:

$$ISI_N\,(D_gP_g) = 2g\left(\frac{3 \times 5}{3+5}\right) + (g+1)\left(\frac{4 \times 4}{4+4}\right) + (8g-6)\left(\frac{4 \times 5}{4+5}\right) + 24g\left(\frac{4 \times 6}{4+6}\right) + 4g\left(\frac{5 \times 5}{5+5}\right) + (4g-6)$$
$$\left(\frac{5 \times 6}{5+6}\right) + 6g\left(\frac{5 \times 7}{5+7}\right) + 18g\left(\frac{6 \times 7}{6+7}\right) + 25g\left(\frac{6 \times 8}{6+8}\right) + g\left(\frac{7 \times 8}{7+8}\right) + 11g\left(\frac{7 \times 9}{7+9}\right) + g\left(\frac{8 \times 9}{8+9}\right)$$
$$= \frac{771121993g}{2450448} - \frac{914}{33}.$$

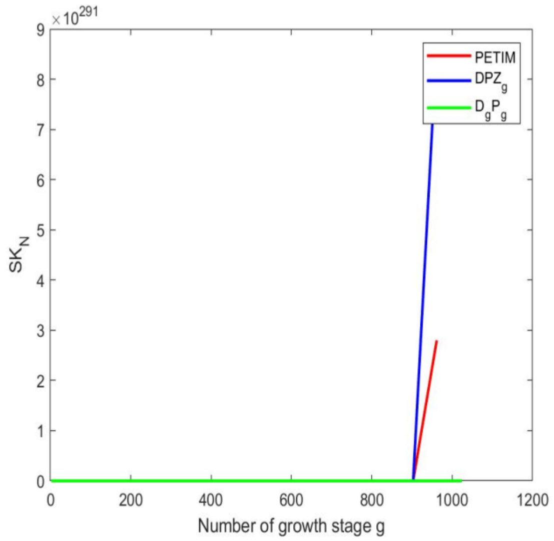


Figure 5. SK_N indexof PETIM, DPZ_g, and D_gP_g dendrimers.

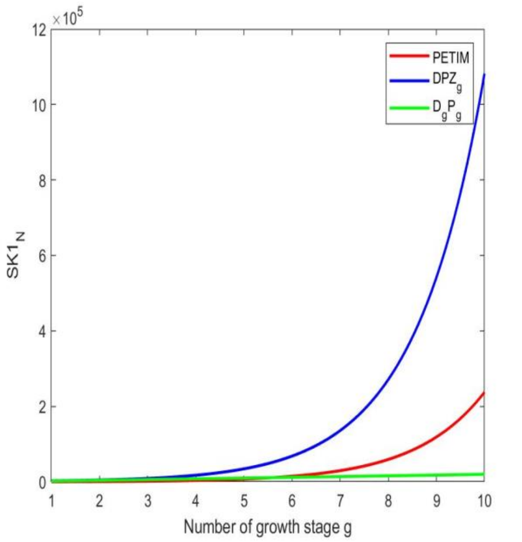
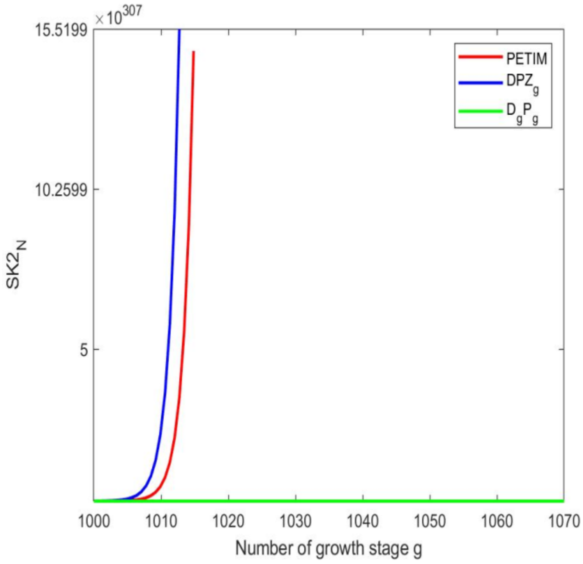


Figure 6. $SK1_N$ index of PETIM, DPZ_g, and D_gP_g.



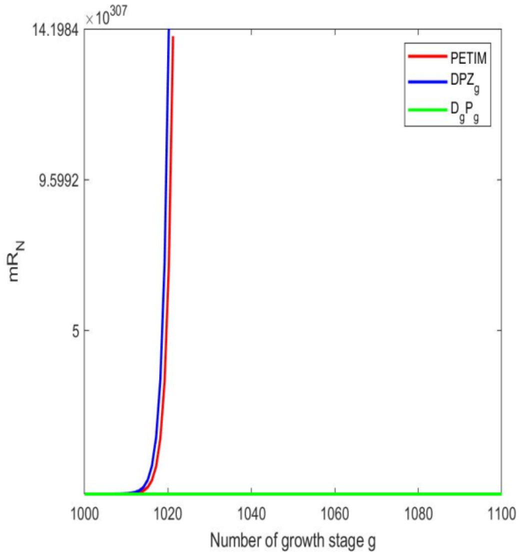


Figure 7. $SK2_N$ index of PETIM, DPZ_g, and D_gP_g dendrimers. **Figure 8.** mR_N index of PETIM, DPZ_g, and D_gP_g

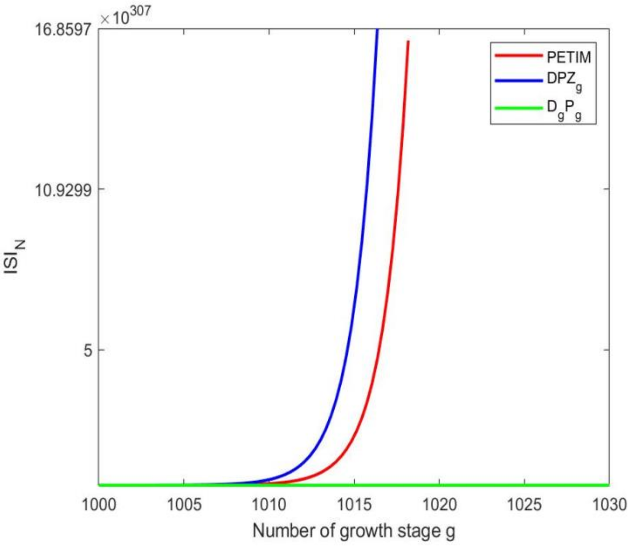


Figure 9. ISI_N indexof PETIM, DPZ_g, and D_gP_g dendrimers.

3.4. Graphical representation.

The graphical representation of SK_N, $SK1_N$, $SK2_N$, mR_N, and ISI_N for the dendrimers PETIM, DPZ_g, and D_gP_g are given in Figure 5-9. In the following figures, the x-axis represents the number of growth-stage g, and the y-axis represents the corresponding index. PETIM, DPZ_g, and D_gP_g dendrimers are plotted by red, blue, and green colors, respectively. It is observed from the figures that DPZ_g has a higher value for Neighborhood-based indices than PETIM and D_gP_g.

4. Conclusions

The molecular study and the research of relation between indices and molecular attributes are made possible by computing numerous topological indices of graphs connected with chemical graphs. In this study, we proposed several Neighborhood-based topological indices for dendrimers, namely PETIM, DPZ_g, and D_gP_g. Chemistry, physics, and other practical disciplines can benefit from our findings. Topological indices have been shown to aid in predicting various properties without the need for a wet lab. MATLAB was also used to illustrate the 2D representations of these indices. We plan to establish the link between these descriptors and various chemical features of dendrimers in the future.

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Conflicts of Interest

The authors declare no conflict of interest.

References

1. Wiener, H. Structural determination of paraffin boiling points. *Journal of the American Chemical Society* **1947**, *69*, 17–20,https://doi.org/10.1021/ja01193a005.
2. Randic, M. Characterization of molecular branching. *Journal of the American Chemical Society* **1975**, *97*, 6609–6615,https://doi.org/10.1021/ja00856a001.
3. Gutman, I. Molecular graphs with minimal and maximal Randic indices. *Croatica Chemica Acta* **2002**, *75*, 357-369,https://hrcak.srce.hr/127525.
4. West, D.B. An Introduction to Graph Theory. 2nded.; Prentice-Hall: New Delhi, India **2002**.
5. Subheet Jain; Amanpreet Kaur; Richa Puri; Puneet Utreja; Anubhuti Jain; Mahesh Bhide; Rakesh Ratnam; Vinay Singh; Patil, A.S.; Jayaraman, N.; Gaurav Kaushik; Subodh Yadav; Khanduja, K.L. Poly propyl ether imine (PETIM) dendrimer: A novel non-toxic dendrimer for sustained drug delivery. *European Journal of Medicinal Chemistry* **2010**, *45*, 4997-5005, https://doi.org/10.1016/j.ejmech.2010.08.006.
6. Lakshminarayanan, A.; Ravi, V.K.; Tatineni, R.; Rajesh, Y. B. R. D.; Maingi, V.; Vasu, K.S.; Madhusudhan, N.; Maiti, P.K.; Sood, A.K.; Das, S.; Jayaraman, N. Efficient Dendrimer–DNA Complexation and Gene Delivery Vector Properties of Nitrogen-Core Poly(propyl ether imine) Dendrimer in Mammalian Cells.*Bioconjugate Chemistry* **2013**, *24*, 1612-1623, https://doi.org/10.1021/bc400247w.
7. Chandan J.; Jayamurugan, G. Structure of poly(propyl ether imine) dendrimer from fully atomistic molecular dynamics simulation and by small angle x-ray scattering.*Journal of Chemical Physics* **2006**, *124*, 204719, https://doi.org/10.1063/1.2194538.
8. Basavaraj K. N.; Hiren M. B.; Ganesh K. D.; Manvi, F.V.; Veerendra K. N. Dendrimers: Emerging polymers for drug-delivery systems.*European Journal of Pharmaceutical Sciences* **2009**, *38*, 185-196,https://doi.org/10.1016/j.ejps.2009.07.008.
9. Astruc, D.; Boisselier, E.; Ornelas, C. Dendrimersdesigned for functions: from physical photophysical and supramolecular properties to applications in sensing catalysis molecular electronics photonics and nanomedicine.*Chemical Reviews* **2010**, *110*, 1857–1959, http://doi.org./10.1021/cr900327d.
10. Humberto G.-D.; Santiago V.; Lourdes S.; Eugenio U. Medicinal Chemistry and Bioinformatics - Current Trends in Drugs Discovery with Networks Topological Indices.*Current Topics in Medicinal Chemistry* **2007**, *7*, 1015-1029, https://doi.org/10.2174/156802607780906771.
11. Yasir B.; Adnan A.; Muhammad K.; Muhammad I. Q.; Adnan J.; Muhammad R.; Nargis B.; Nazeer M.On Forgotten Topological Indices of Some Dendrimers Structure. *Molecules* **2017**, *22*, 867, https://doi.org/10.3390/molecules22060867.
12. Alyar, S.; Khoeilar, R.; Jahanbani, A. Some topological indices of dendrimers. *International Journal of Computational Materials Science and Engineering* **2020**, *9*, 2050018, http://doi.org/10.1142/S2047684120500189.
13. Kang, S.M.; Zahid, M.A.; Virk,A.R.; Nazeer, W.; Gao, W. Calculating the Degree-based Topological Indices of Dendrimers.*Open Chemistry* **2018**, *16*, 681-688, https://doi.org/10.1515/chem-2018-0071.
14. Gao, W.; Aamir, M.; Iqbal, Z.; Ishaq, M.; Aslam, A. On Irregularity Measures of Some Dendrimers Structures. *Mathematics* **2019**, *7*, 271, https://doi.org/10.3390/math7030271.
15. Aslam, A.; Jamil, M.K.; Gao, W.; Nazeer, W. Topological aspects of some dendrimer structures.*Nanotechnology Reviews* **2018**, *7*, 123-129, https://doi.org/10.1515/ntrev-2017-0184.
16. Shahid A.; Abaid R.V.; Rehman, M.A.; Nehad A.S. Analysis of Dendrimer Generation by Sombor Indices.*Journal of Chemistry* **2021**, *2021*,11, https://doi.org/10.1155/2021/9930645.
17. Aslam, A.; Bashir, Y.; Rafiq, M.; Haider, F.; Muhammad, N.; Bibi, N. Three New/Old Vertex-Degree Based Topological Indices of some Dendrimers Structure. *Electronic Journal of Biology* **2017,** *13*.

18. Diudea, M.; Vizitiu, A.; Mirzagar, M.; Ashrafi, A. Sadhana polynomial in nano-dendrimers. *Carpathian Journal of Mathematics* **2010**, *26*, 59-66, https://www.jstor.org/stable/43999432.
19. Zhihua C.; Abaid R.V.; Mustafa H.; Tariq J.Z.; Imran A.; Ce S.; Waqas N. Irregularity Indices of Dendrimer Structures Used as Molecular Disrupter in QSAR Study. *Journal of Chemistry* **2019**, *2019*, 21, https://doi.org/10.1155/2019/5371254.
20. Chu, Z.-Q.; Salman, M.; Munir, A.; Khalid, I.; Rehman, M.U.; Liu, J.-B.; Ali, F. Some topological indices of dendrimers determined by their Banhatti polynomials. *Heterocyclic Communications* **2020**, *26*, 99-111, https://doi.org/10.1515/hc-2020-0102.
21. Murat C.; Süleyman E.; Hafiz M.-U.-R.; Deeba A. M-polynomial and topological indices Poly (EthyleneAmidoAmine) dendrimers. *Journal of Information and Optimization Sciences* **2020**, *41*, 1117-1131, http://doi.org./10.1080/02522667.2020.1745383.
22. Modjtaba G.; Mina R.-P.; Ottorino O. Distance complexity measures versus the orbit-entropy measure of dendrimers. *Fullerenes, Nanotubes and Carbon Nanostructures* **2021**, https://doi.org/10.1080/1536383X.2021.1955246.
23. Mondal, S.; De, N.; Pal, A. Neighborhood degree sum-based molecular descriptors of fractal and Cayley tree dendrimers. *European Physical Journal Plus* **2021**, *136*, 303, https://doi.org/10.1140/epjp/s13360-021-01292-4.
24. Mathad, V.; Padmapriya, P.; Sangamesha, M.A.Some topological indices of phosphorus containing dendrimers. *Palestine Journal of Mathematics* **2021**, *10*, 151-160.
25. Muhammad K.H.; Faryal C.; Abdul J.M.; Khalaf, M.; Reza F. Investigation of dendrimer structures by means of reverse atomic bond connectivity index. *Journal of Discrete Mathematical Sciences and Cryptography* **2021**, *24*, 473-485, http://doi.org/10.1080/09720529.2021.1882161.
26. Nur H.A.M.S.; Mohamad N.H.; Nur B.I. On the zagreb indices of the line graphs of polyphenylene dendrimers. *Journal of Discrete Mathematical Sciences and Cryptography* **2020**, *23*,1239-1252, http://doi.org/10.1080/09720529.2020.1822041
27. Khalaf, A.J.M.; Javed, A.; Jamil, M. K.; Alaeiyan, M.; Reza F.M. Topological properties of four types of porphyrin dendrimers. *Proyecciones* **2020**, *39*, 979-993, https://doi.org/10.22199/issn.0717-6279-2020-04-0061.
28. Iqbal, Z.; Aslam, A.; Ishaq, M.; Gao, W. The Edge Versions of Degree-Based Topological Descriptors of Dendrimers. *Journal of Cluster Science* **2020**, *31*, 445-452, https://doi.org/10.1007/s10876-019-01658-w.
29. Pattabiraman, K.; Santhakumar, A.; Satheeshkumar, G. Degree based descriptors of certain classes of dendrimer graphs. *Materials Today: Proceedings* **2021**, *42*, 1258-1261, https://doi.org/10.1016/j.matpr.2020.12.881.
30. Buragohain, J.; Deka, B.; Bharali, A. A generalized ISI index of some chemical structures. *Journal of Molecular Structure* **2020**, *1208*, 127843, https://doi.org/10.1016/j.molstruc.2020.127843.
31. Gao, W.; Iqbal, Z.; Jaleel, A.; Aslam, A.; Ishaq, M.; Aamir, M. Computing entire Zagreb indices of some dendrimer structures. *Main Group Metal Chemistry* **2020**, *43*, 229-236, https://doi.org/10.1515/mgmc-2020-0027.
32. Gao, W.; Akhter, S.; Iqbal, Z.; Qasim, M.; Aslam, A. The Topological Aspects of Phthalocyanines and Porphyrins Dendrimers. *IEEE Access* **2020**, *8*, 168631-168649, https://doi.org/10.1109/ACCESS.2020.3023658.
33. Vignesh R.; Kalyani D.Neighbourhood Degree - Based Topological Indices of Graphene Structure. *Biointerface Research in Applied Chemistry***2021**, *11*, 13681-13694, https://doi.org/10.33263/BRIAC115.1368113694.
34. Sourav M.; Nilanjan D.; Anita P. On some New Neighbourhood Degree Based Indices.*Acta Chemica Iasi* **2019**, *27*, 1, 31-46, https://doi.org/10.2478/achi-2019-0003.
35. Sourav M.; Nilanjan D.; Anita P. Topological properties of Graphene using some novel neighborhood degree-based topological indices.*International Journal of Mathematics for Industry* **2019**, *11*, 1950006, http://doi.org/10.1142/S2661335219500060.
36. Mondal, S.; De, N.; Pal, A. On Some New Neighborhood Degree-Based Indices for Some Oxide and Silicate Networks. *J Multidisciplinary Scientific Journal* **2019**, *2*, 384-409, https://doi.org/10.3390/j2030026.
37. Shanmukha, M.C.; Basavarajappa, N.S.; Usha, A.; Shilpa, K.C. Novel neighborhood redefined first and second Zagreb indices on carborundum structures. *Journal of Applied Mathematics and Computing* **2021**, *66*, 263-276, https://doi.org/10.1007/s12190-020-01435-3.
38. Mondal, S.; Dey, A.; De, N.; Pal, A. QSPR analysis of some novel neighborhood degree-based topological descriptors. *Complex and Intelligent Systems* **2021**, *7*, 977-996, https://doi.org/10.1007/s40747-020-00262-0.
39. Syed A. K. K.; Parvez A.; Faizul A. Topological indices and QSPR/QSAR analysis of some antiviral drugs being investigated for the treatment of COVID-19 patients. *International Journal of Quantum Chemistry* **2021**, *121*, 1-22, https://doi.org/10.1002/qua.26594.
40. Sourav M.; Nilanjan D.; Anita P. On neighborhood Zagreb index of product graphs. *Journal of Molecular Structure* **2021**, *1223*, 129210, https://doi.org/10.1016/j.molstruc.2020.129210.