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Leap Edge Eccentricity Connectivity Index of PAMAM and Porphyrin-Cored Dendrimers

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Abstract

With the rapid advancement of technology, computer-aided methods are increasingly employed to study the structural properties of chemical compounds. One such approach involves predicting chemical behavior using topological indices—numerical descriptors derived from graph-theoretic representations of molecular structures.

In this paper, the leap edge eccentricity connectivity index is introduced distance-based topological index that can be regarded as both the edge version of the leap eccentric connectivity index and the leap version of the edge eccentric connectivity index and investigates the leap edge eccentricity connectivity index (LEECI) for Polyamidoamine (PAMAM) dendrimers and porphyrin-cored dendrimers through exact analytical computations. By modeling these nanostructures with graphs, LEECI values for multiple dendrimer structures are derived. The results reveal strong correlations between branching complexity and index growth, highlighting LEECI as a promising descriptor in computational nanomaterial characterization and drug delivery design. These findings provide a foundation for integrating LEECI into predictive models linking molecular topology with experimental properties.

Keywords: Graph Theory, Topological index, Leap edge eccentricity connectivity index, Dendrimer Graphs.
2010 MSC: 05C90, 05C92, 05C09, 92E10.

1. Introduction

Due to evolving living conditions and increasing disease prevalence, there is a growing demand for rapid and cost-effective methods for the discovery of novel chemicals and pharmaceuticals. With the aid of topological indices in chemical graph theory, it is now possible to predict the physical, chemical, and biological properties of molecular structures. These indices are mathematical values derived from molecular graphs,

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which represent molecular structures through vertices and edges: non-hydrogen atoms are represented as vertices, and chemical bonds between atoms as edges.

Topological indices, based on graph properties such as degree, energy, and distance, are used to establish quantitative relationships between the structure and properties of molecules [17]. Among the most studied are degree-based indices.The number of graph indices based on the degree of vertices is much larger due to their easy calculation, and the first of them are the first Zagreb index and is defined as follows [8]:

$$M_1(\Phi) = \sum_{\tilde{u} \in V(\Phi)} d(\tilde{u})^2 = \sum_{\tilde{u}\tilde{v} \in E(\Phi)} (d(\tilde{v}) + d(\tilde{u})) = \sum_{\tilde{v} \in V(\Phi)} \sum_{\tilde{v} \in N(\tilde{u})} d(\tilde{v})$$

Later extended into a leap version by Naji et al, in 2017, Naji et al [12] defined as

$$LM_3(\Phi) = \sum_{\tilde{v}\tilde{u} \in E(\Phi)} (d_2(\tilde{v}) + d_2(\tilde{u}))$$

In 2012, Ghorbani and Hosseinzadeh [7] defined eccentric version of the first Zagreb index as

$$\xi^c(\Phi) = \sum_{\tilde{v}\tilde{u} \in E(\Phi)} (\varepsilon(\tilde{u}) + \varepsilon(\tilde{v}))$$

Sharma et al. proposed eccentric connectivity index in 1997 as [15]

$$\xi^c(\Phi) = \sum_{\tilde{v} \in V(\Phi)} d(\tilde{v})\varepsilon(\tilde{v}) \tag{1.1}$$

Xu and Guo introduced edge version of eccentric connectivity index in 2012 [18]

$$\xi^c_e(\Phi) = \sum_{f \in E(\Phi)} d(f)\varepsilon(f) \tag{1.2}$$

After, The leap version of Sharma's index is independently introduced by in [13], Manjunathe et al. [11], and Ghalavand et al. [6] as

$$L\xi^c(\Phi) = \sum_{\tilde{v} \in V(\Phi)} d_2(\tilde{v})\varepsilon(\tilde{v}) \tag{1.3}$$

Dendrimers are nanoscale, highly branched, three-dimensional polymeric materials that resemble tree graphs. Their potential applications in drug delivery, particularly in the treatment of cancer, neurodegenerative diseases, and central nervous system (disorders, are widely recognized [1]. Dendrimers offer promising avenues for efficient molecular delivery due to their unique chemical properties. Previous works have explored various topological characteristics of dendrimers, including irregularity indices [19], M-polynomials [9], generalized Zagreb indices [14], and degree-based indices [10].

While several degree- and distance-based indices have been investigated for dendrimers, the leap edge eccentricity connectivity index remains unexplored in this context. This study addresses this gap by providing exact formulations for PAMAM and porphyrin-cored dendrimers, enabling direct structural comparisons.

In this paper, it is computed and compared the leap edge eccentricity connectivity indices of molecular graphs of polyamidoamine (PAMAM) dendrimers, porphyrin Cored Dendrimer-2, -3, and -4.

2. Preparation

Let G be a chemical graph. In a graph G, the degree of a vertex v, denoted by $d(v)$, is the number of edges adjacent to v. The 2-distance degree of a vertex v, denoted by $d_2(v)$, is the number of vertices at distance two from v. The eccentricity of a vertex v in a connected graph G, denoted by $\varepsilon(v)$, is the maximum distance from v to any other vertex in G [3]. If $e = u_1u_2$ and $f = v_1v_2$ are two edges of G, then distance between e and f is $d(e, f) = min\{d(u_1, v_1), d(u_1, v_2), d(u_2, v_1), d(u_2, v_2)\} + 1$ [4].

Polyamidoamine (PAMAM) dendrimers consist of an ethylenediamine core, a repeating branched amidoamine internal structure, and primary amine terminal surfaces [5]. Let PAMAM[r] denote the molecular graph of a PAMAM dendrimer with r generations. Figure 1(a) shows the chemical structure of a PAMAM dendrimer with 3 generations [16], while Figure 1(b) illustrates its corresponding graph $PAMAM[3]$. PAMAM dendrimer graphs with r generations have $|V(PAMAM[r])| = 12 \times 2^{r+2} - 23$ and $|E(PAMAM[r])| = 12 \times 2^{r+2} - 24$. Porphyrin-cored dendrimers consist of a central core and at least two branches. In the graph

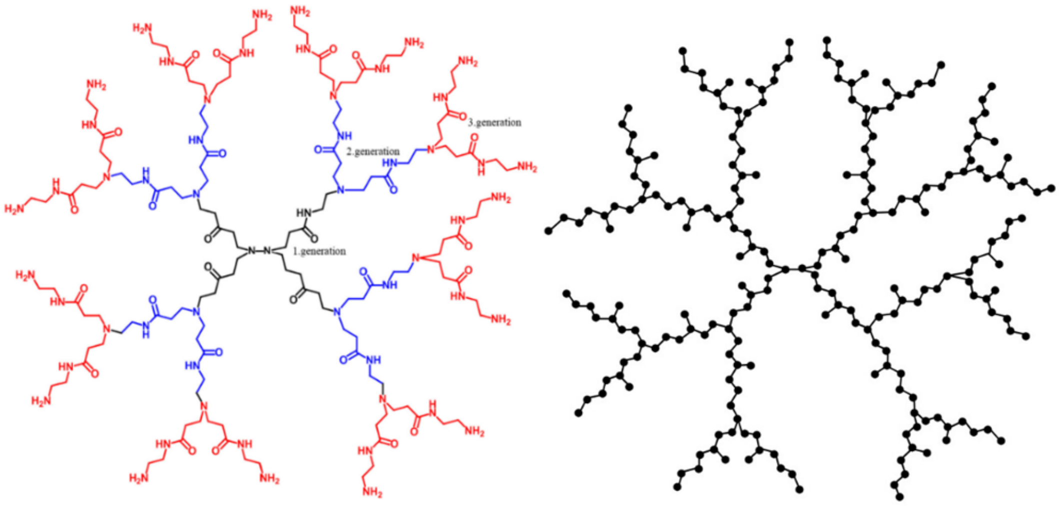

Figure 1: (a) PAMAM dendrimer with 3 generations (b) its graph representation.

of such dendrimers, the central core includes 25 vertices and 36 edges.

Porphyrin core dendrimers-2 (Porphyrin core dendrimers-2) have a central core and 4 branches. Figure 2 shows the structure of porphyrin core dendrimers-2 (D4) [2]. Let the molecular graph of porphyrin core dendrimers-2 be denoted by $PC2[n]$ for $1 \leq n$. Let n denote dendron-like arms. Therefore, since the dendrimer in Figure 2 has 4-dendron-like arms, the graph of this structure is $PC2[n]$. Porphyrin core dendrimers-3 have a central core and 8 branches. Assume that $PC3[n]$ for $1 \leq n$ denote the molecular graph of porphyrin core dendrimers-3. Here n denotes dendron-like arms. Figure 3 shows the structure of porphyrin core dendrimers-3 having 3 dendron-like arms (D3) [2]. Porphyrin core dendrimers-4 has a central core and 12 branches. Assume that $PC4[n]$ for $1 \leq n$ denote the molecular graph of porphyrin core dendrimers-4. Figure 4 shows the structure of porphyrin core dendrimers-4 [2].

3. Main Results

In this section, the leap edge eccentricity connectivity index (LEEC) is introduced and then LEEC of the molecular graphs of the PAMAM dendrimer, porphyrin cored dendrimer-2, porphyrin cored dendrimer-3, and porphyrin cored dendrimer-4 are obtained and numerically compared.

With the motivation of Equations ((1.1)-(1.3)), the leap edge eccentric connectivity index is introduced as

$$L\xi_e^c(\Phi) = \sum_{f \in E(\Phi)} d_2(f)\epsilon(f) \tag{3.1}$$

where $\epsilon(f) = max\,\{d(f, f_1)\,|f_1 \in E(\Phi)\}$ and $d_2(f) = |\{f_1 \in E(\Phi)\,|d(f, f_1) = 2\}|$.

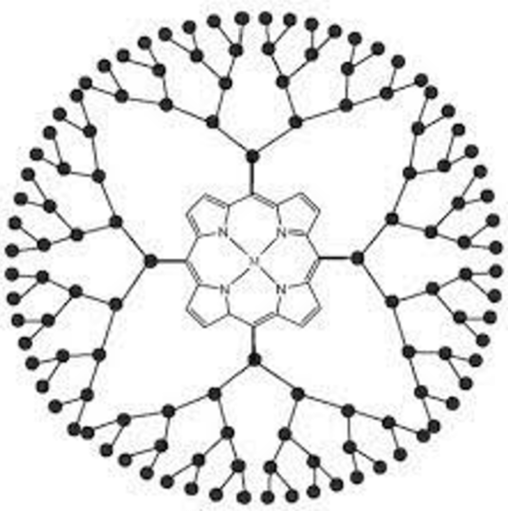

Figure 2: Porphyrin Cored Dendrimer-2.

Example 3.1. Let G be a graph with 7 vertices and 8 edges as shown in the Figure 5. Leap edge eccentricity connectivity index of G is 56.

Proof. From Figure 5 the following Table 1 is obtained. For $e_1 \in E$, $d_2(e_1) = |\{e_3, e_6, e_7\}| = 3$. From Eq.

Edge	$d_2(f)$	$\varepsilon(f)$
e_1	3	3
e_2	3	2
e_3	4	2
e_4	2	3
e_5	3	3
e_6	2	2
e_7	3	2
e_8	4	2

Table 1: Edge decomposition of the graph.

(3.1), this proof is completed. □

Theorem 3.2. *Let $PC2[n]$ be the graph of the porphyrin cored dendrimer-2. Then, the leap edge eccentricity connectivity index of $PC2[n]$ for $2 \leq n$ is given by:*

$$L\zeta_e^c(PC2[n]) = 216n + 1140 + 2^{n+3}(4n + 13) + 32\sum_{i=2}^{n} 2^{n-i}(2n + 7 - i)$$

Proof. As seen in Figure 2, the core of $PC2[n]$ has 32 edges and each branch contains $\sum_{j=0}^{n} 2^j$ edges. From Eq. (3.1), it is obtained the expression:

$$L\zeta_e^c(PC2[n]) = \sum_{Core} \varepsilon(e)\, d_2(e) + 4 \sum_{Branch} \varepsilon(e)\, d_2(e) \tag{3.2}$$

The 2-distance degree and edge eccentricity values in the core and one branch are given in Table 2 and Table 3, respectively.

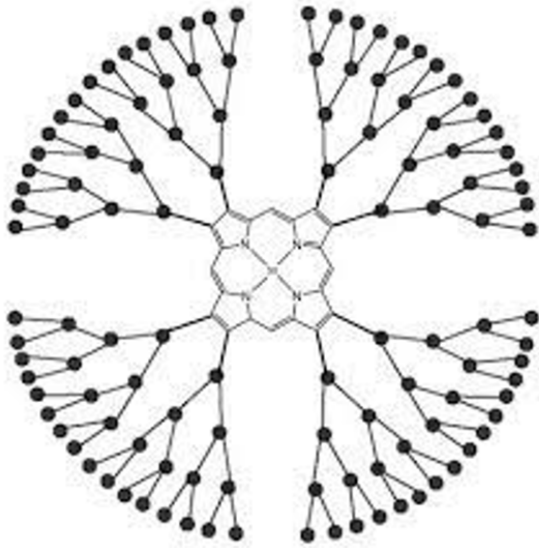

Figure 3: Porphyrin Cored Dendrimer-3.

$d_2(f)$ **for E(PC2[n])**	$\varepsilon(f)$ **for E(PC2[n])**	**Number of edges**
4	n+7	4
5	n+6	8
7	n+6	4
7	n+5	4
8	n+5	8
10	n+4	4

Table 2: Edge decomposition of the graph of the core structure according to 2-distance degrees and eccentric distances.

If the data in Table 2 and Table 3 are used in Eq. (3.2), the following equations are obtained:

$$\sum_{Core} \varepsilon(e)d_2(e) = 4(n+7)4 + 8(6+n)5 + 4(n+6)7 + 4(n+5)7$$
$$+8(n+5)8 + 10(n+4)4 = 216n + 1140 \tag{3.3}$$

$$\sum_{Branch} \varepsilon(e)\, d_2(e) = 2^n\,(2(2n+7)) + 2^{n-1}\,(4(2n+6)) + 8\sum_{i=2}^{n} 2^{n-i}(2n+7-i) \tag{3.4}$$

The proof is completed from Equations (3.2), (3.3) and (3.4). The graphic of the leap edge eccentricity connection index of the graph is given in Figure 6.

□

Theorem 3.3. *Let $PC3[n]$ be the graph of the porphyrin cored dendrimer-3. Then, the leap edge eccentricity connectivity index of $PC3[n]$ for $n \geq 2$ is given by:*

$$L\zeta_e(PC3[n]) = 240n + 1328 + 2^{n+4}(4n+13) + 64\sum_{i=2}^{n} 2^{n-i}(2n+7-i)$$

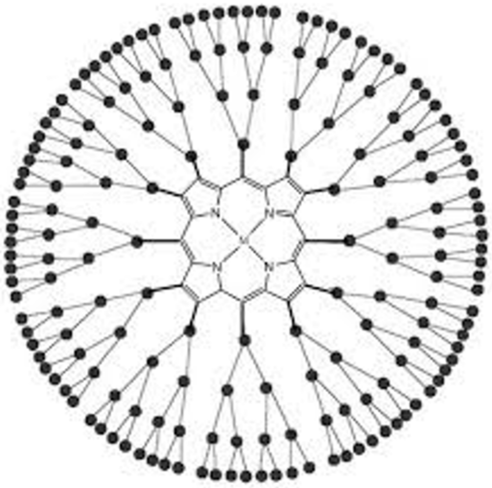

Figure 4: Porphyrin Cored Dendrimer-4.

$d_2(f)$ **for E(PC2[n])**	$\varepsilon(f)$ **for E(PC2[n])**	**Number of edges**
2	2n+7	2^n
4	2n+6	2^{n-1}
8	2n+5	2^{n-2}
8	2n+4	2^{n-3}
...	...	...
8	n+7	2^1
8	n+6	2^0

Table 3: Edge decomposition on a branch of a porphyrin dendrimer-2.

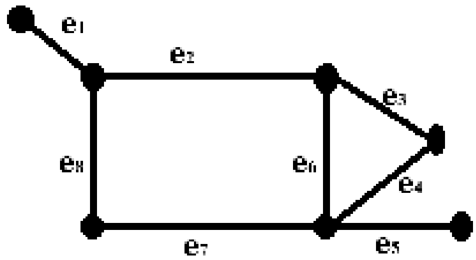

Figure 5: Graph Example.

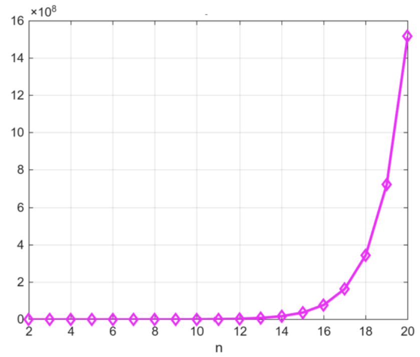

Figure 6: Graphic of $L\zeta_e^c(PC2[n])$.

Proof. As shown in Figure 3, the core of $PC3[n]$ also has 32 edges and each branch has a similar structure to those in $PC2[n]$. By analyzing the structure and using Eq. (3.1), it is obtained the result.

$$L\zeta_e^c(PC3[n]) = \sum_{Core} \varepsilon(e)\, d_2(e) + 8 \sum_{Branch} \varepsilon(e)\, d_2(e) \tag{3.5}$$

The two-distance degree depending on the edge in the core of the $PC3[n]$ graph and the edge separation of that edge according to the edge eccentricity are given in Table 4.

$d_2(f)$ **for** $E(PC3[n])$	$\varepsilon(f)$ **for E(PC3[n])**	**Number of edges**
8	n+7	4
7	n+6	8
6	n+6	8
8	n+5	8
10	n+4	4

Table 4: Edge separation of the core structure of the $PC3[n]$.

Then

$$\sum_{Core} \varepsilon(e)d_2(e) = 4(8(n+7)) + 8(6+n)7 + 8(n+6)6 + 8(n+5)8 + 10(n+4)4$$
$$= 240n + 1328 \tag{3.6}$$

Since the edge partitions and branch structures are the same as in $PC2[n]$, from Eq. (3.4)-(3.6), it is concluded that:

$$L\zeta_e(PC3[n]) = 240n + 1328 + 8\left[2^n\left(2(2n+7)\right) + 2^{n-1}\left(4(2n+6)\right) + 8\sum_{i=2}^{n} 2^{n-i}(2n+7-i)\right]$$

Figure 7 shows the graph of the leap edge eccentric connection index of $PC3[n]$ graphs.

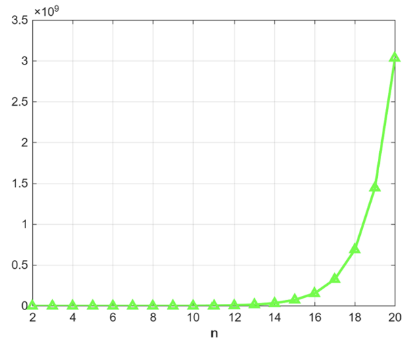

Figure 7: The graph of the LEECI for $PC3[n]$.

□

Theorem 3.4. *Let $PC4[n]$ be the graph of the porphyrin cored dendrimer-4. Then, the leap edge eccentricity connectivity index of $PC4[n]$ for $n \geq 2$ is given by:*

$$L\zeta_e(PC4[n]) = 272n + 1512 + 2^{n+3}(12n+39) + 96\sum_{i=2}^{n} 2^{n-i}(2n+7-i)$$

Proof. $PC4[n]$ has 12 branches and a central core. From Figure 4, the core has 32 edges, and each branch has the same structure as in $PC2[n]$. Table 5 shows the edge partitioning according to the 2-distance degrees of the core and the eccentric distances of the edges.

$d_2(f)$ **for** $E(PC4[n])$	$\varepsilon(f)$ **for** $E(PC4[n])$	**Number of edges**
8	n+6	16
8	n+7	4
9	n+5	8
10	n+4	4

Table 5: Edge decomposition in the core of the graph $PC4[n]$.

Using Table 5, Eq. (3.1) and Eq.(3.4), it is computed:

$$\begin{aligned} L\zeta_e(PC4[n]) &= 272n + 1512 + 12(2^n\left(2(2n+7)\right) + 2^{n-1}\left(4(2n+6)\right) \\ &+ 8\sum_{i=2}^{n} 2^{n-i}(2n+7-i)) \end{aligned}$$

Figure 8 shows the graph of the equation $L\zeta_e(PC4[n])$.

□

Theorem 3.5. *Let $PAMAM[r]$ be the graph of the PAMAM dendrimer. Then, the leap edge eccentricity connectivity index of $PAMAM[r]$ is given by:*

$$L\zeta_e^c(PAMAM[r]) = 70r + 16 + 2^{r+1}(252r-31) + \sum_{i=1}^{r-1} 2^{r+1-i}(308r-25+154i)$$

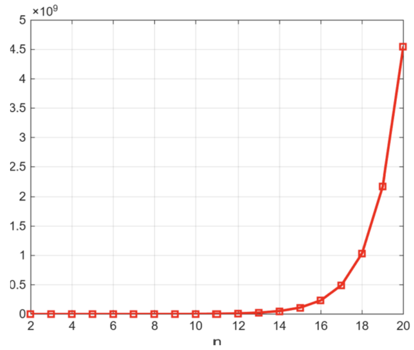

Figure 8: The graph of the LEECI for $L\zeta_e^c(PC4[n])$.

Proof. The PAMAM dendrimer graph has 3 edges in the core and 4 branches. There are $\sum_{i=1}^{r} 2^{i+2}$ edges in each branch. From Eq. (3.1), ıt is obtained that

$$L\zeta_e^c(PAMAM[r]) = \sum_{Core} \varepsilon(e)d_2(e) + \sum_{i=1}^{r-1} 2^{i+1} \sum_{Branch} \varepsilon(e)d_2(e) + 2^{r+1} \sum_{Branch} \varepsilon(e)d_2(e) \tag{3.7}$$

The two-distance edge degree and edge eccentricity numbers of the three vertices in the core are shown in Table 6.

$d_2(f)$	$\varepsilon(f)$
3	$2+7r$
4	$1+7r$
3	$2+7r$

Table 6: The two-distance edge degree and edge eccentricity numbers of the three vertices in the core.

There are 4 branches in the $PAMAM[1]$ graph with extension $r = 1$. There is a tree structure of length 7 with 8 vertices in one branch. The two-distance edge degree and edge eccentricity of the edges in the r extension in the $PAMAM[r]$ graph are given in Table 7.

$d_2(f)$	$\varepsilon(f)$
1	$2+14r$
1	$1+14r$
3	$14r$
2	$14r-1$
2	$14r-2$
2	$14r-2$
4	$14r-3$
3	$14r-4$

Table 7: Two-distance edge degree and edge eccentricity in a branching r extension.

The edge decomposition in a branch of the graph $PAMAM[r]$ in each extension i in the extensions $1 \le i \le r-1$ is given in Table 8.

If the data in Tables 6, 7 and 8 are used in Eq. (3.7), the following equation is obtained:

$d_2(f)$	$\varepsilon(f)$
3	$2-7i+14r$
3	$1-7i+14r$
3	$14r-7i$
2	$14r-1-7i$
2	$14r-2-7i$
2	$14r-2-7i$
4	$14r-3-7i$
3	$14r-4-7i$

Table 8: Two-distance edge degree and edge epicenter of a branch in branching i.

$$\begin{aligned}
L\zeta_e(PAMAM[r]) &= 70r+16+2^{r+1}(252r-31)\\
&+ \sum_{i=1}^{r-1} 2^{r+1-i}(3(14r+2-7i)+3(14r+1-7i)\\
&+ 3(14r-7i)+2(14r-1-7i)+2(14r-2-7i)\\
&+ 2(14r-2-7i)+4(14r-3-7i)+3(14r-4-7i)).
\end{aligned}$$

Figure 9 shows the graph of the leap edge eccentric connection index of the graph of PAMAM dendrimer.

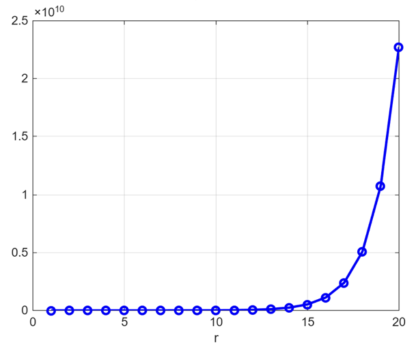

Figure 9: Graph of the LEECI for $PAMAM[r]$.

□

4. Conclusion

Today, predicting the properties of chemical structures using computer-aided methods has become increasingly important. By modeling chemicals as graphs and applying graph-theoretical concepts, numerical results obtained from these graphs can be used to predict the characteristics of the corresponding molecules.

In this study, it is calculated the leap edge eccentricity connectivity indices of the molecular graphs of three porphyrin-cored dendrimers and one PAMAM dendrimer. Figure 10 presents the LEECI values for Porphyrin Cored Dendrimer-2, -3, and -4.

As shown in Figure 10, the dendrimer with the highest number of branches and edges exhibits the highest LEECI value. Figure 11 compares the LEECI values of the PAMAM dendrimer and the three porphyrin-cored dendrimers.

Figure 11 clearly indicates that the LEECI value for the PAMAM dendrimer increases at a significantly higher rate than those of the porphyrin-cored dendrimers as the number of branches increases.

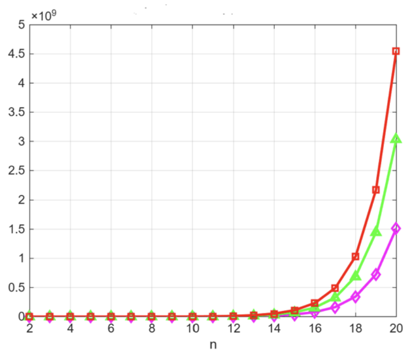

Figure 10: Leap edge eccentric connectivity indices of porphyrin core dendrimer graphs.

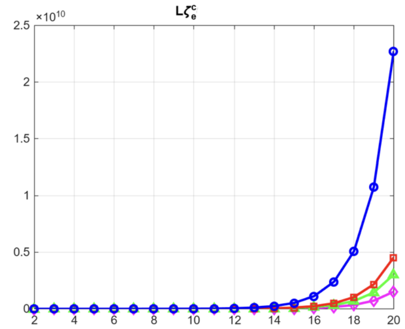

Figure 11: Dendrimer graphs according to index values.

These findings indicate that the LEECI is highly sensitive to changes in dendrimer branching patterns, making it a promising descriptor for predicting the structural and functional properties of nanoscale macromolecules. Future work may focus on correlating LEECI values with experimental biological activity and physicochemical data to further validate its applicability in drug design.

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