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Comparison of Irregularity Indices of Several Dendrimers Structures

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Abstract: Irregularity indices are usually used for quantitative characterization of the topological structures of non-regular graphs. In numerous problems and applications, especially in the fields of chemistry and material engineering, it is useful to be aware of the irregularity of a molecular structure. Furthermore, the evaluation of the irregularity of graphs is valuable not only for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies but also for various physical and chemical properties, including entropy, enthalpy of vaporization, melting and boiling points, resistance, and toxicity. In this paper, we will restrict our attention to the computation and comparison of the irregularity measures of different classes of dendrimers. The four irregularity indices which we are going to investigate are σ irregularity index, the irregularity index by Albertson, the variance of vertex degrees, and the total irregularity index.

Keywords: molecular graph; irregularity indices; dendrimers

1. Introduction

The rapid growth in the field of medicine has resulted in the production of unknown nanomaterials, crystalline materials, and drugs. To investigate the chemical properties of these compounds, huge efforts of the pharmaceutical researchers are required and are being made. One way to understand it is by using mathematics, and in mathematical chemistry many concepts of graph theory are being used to formulate the mathematical models for chemical phenomena. Molecules and molecular compounds can be considered as graphs if we correspond atoms to vertices and chemical bonds to edges respectively. Such graphs are called molecular graphs. The notion of topological indices (TIs) helps the pharmacists by providing some information based upon the structures of materials, which reduce their workload. Computing the TIs of a compound may help in approximating its medicinal behaviour [1]. With the passage of time, the idea of understanding compounds through TIs gained significant importance in the field of medicine because it does not require chemical-related apparatus to study [2]. TIs are being intensively studied for different graphs, especially for chemical graphs, for example, see [3–6]. TIs can be separated into various classes, specifically distance-based indices, degree-based indices, eigenvalue-based indices, and mixed indices. An important subclass

of degree-based indices is the class of irregularity indices that measure the irregularity of the given graph. A topological invariant $TI(G)$ of a graph G is known as the irregularity index if $TI(G) \geq 0$ and $TI(G) = 0$, if and only if, it is a regular graph. Before the article [7], it was considered that the irregularity indices do not play a significant role to predict physico-chemical properties of organic molecules. In [7] authors performed a regression analysis to check and evaluate the applications of different graph irregularity indices for the estimation of physico-chemical properties of octane isomers. They showed that there exist many irregularity indices by which four octane isomer properties such as standard enthalpy of vaporization (DHVAP), Acentric factor (AcenFac), Entropy, and Enthalpy of vaporization (HVAP) can be estimated with a correlation coefficient greater than 0.9. Before proceeding further with the details related to irregularity indices, we include some important definitions.

Throughout the article, we denote vertex set of a graph G by $V(G)$ and edge set by $E(G)$. A regular graph is a graph whose all vertices have the same degree, otherwise it is called the irregular graph. A sequence $c_1, \ldots, c_{n'}$, where $c_i \in \mathbb{Z}^+$ for all $i = 1, \ldots, n'$, is called a degree sequence of a graph G, if a graph G exists with the property that $V(G) = \{v_1, \ldots, v_{n'}\}$ and $d_G(v_j) = c_j$. Let n_j denotes the number of vertices of degree j, where $j = 1, 2, \ldots, n-1$. Let $e = uv \in E(G)$, the imbalance of e is defined as $imb(e) := |d_G(u) - d_G(v)|$. In 1997, the term "irregularity of a graph G" was introduced by Albertson [8]. It is denoted by $irr(G)$ and defined as follows:

$$irr(G) = \sum_{e \in E(G)} imb(e) \tag{1}$$

This invariant is also known as the third Zagreb index. It follows immediately that a graph has zero irregularity if and only if it is a regular graph. Albertson [8] showed that the irregularity of any graph is an even number. Furthermore, he also proposed upper bounds for irregularity of triangle-free graphs, bipartite graphs, and for trees. The relationships between the matching number and irregularity of unicyclic graphs and trees were examined in [9]. Hansen et al. [10] characterized the graphs with maximal irregularity. Abdo and Dimitrov [11] worked out for the irregularity of graph operations. In 2014, Abdo et al. [12] defined the total irregularity measure of a graph G, which was denoted and detailed as follows:

$$irr_t(G) = \frac{1}{2} \sum_{u,v \in V(G)} |d_G(u) - d_G(v)|. \tag{2}$$

The relationship between irregularity measures, characterization of graphs with extremal irregularity and the smallest graph with the same irregularity indices are explored in [13]. Fath-Tabar [14] set up some new bounds on the Zagreb indices using the irregularity of graphs. For the detail discussions about these graph invariants, we refer [15,16]. Very recently, Gutman et al. [17] introduced the σ irregularity index of a graph G, which is described as:

$$\sigma(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2. \tag{3}$$

Some properties of this index have been presented in [18,19]. If the order and size of G is n and m, then the variance of G is defined as [20]:

$$Var(G) := \frac{1}{n} \sum_{j=1}^{n-1} n_j \left(j - \frac{2m}{n}\right)^2 = \frac{1}{n} \sum_{j=1}^{n} d_j^2 - \frac{1}{n^2} \left(\sum_{j=1}^{n} d_j\right)^2. \tag{4}$$

As for prerequisite, the reader is expected to be familiar with dendrimers. Recently, it has been noticed that the highly branched macromolecules have exceptionally different properties from the traditional polymers. Their structural properties have a huge impact on their applications. These hyperbranched molecules are called dendrimers. Moreover, the linear growth in the size

of dendrimers makes them the ideal delivery vehicle candidates for the study of effects of composition, and size of polymer in the biological properties like cytotoxicity, blood plasma retention time, lipid bilayer interactions, and filtration, see [21] and references therein. These molecules were first discovered (and studied) by E.Buhleier [22], D. Tomalia [23], and G. R. Newkome [24]. There are many known dendrimers with biological properties such as chemical stability, solubility, polyvalency, electrostatic interactions, low cytotoxicity and self-assembling.

Although plenty of work has been executed on the distance and degree based indices of molecular graphs, the analyses of irregularity measures for chemical structures still need attention. In [25–28], the irregularity measures of various chemical structures were investigated. In this work, we are interested in the irregularity indices of the molecular graphs of different types of dendrimers. For some topological aspects of different complex dendrimers structures, we refer the interested reader to [29–37]. We will restrict our attention to three dendrimers Polyamidoamine (PAMAM), Poly(EThyleneAmidoAmine) (PETAA), and poly(PropylETherIMine)(PETIM) dendrimers.

2. Main Results

In this section, we will compute the irregularity indices of several classes of dendrimers. Firstly, we describe the significance of PAMAM dendrimers. Furthermore, we will also compute four irregularity indices for PAMAM dendrimers.

2.1. Irregularity Measures of PAMAM Dendrimers

The PAMAM dendrimers are a family of dendrimers which is made of repetitively branched subunits of amide and amine functionality. PAMAM dendrimers have hydrophilic interiors and exteriors, which play a role for its unimolecular micelle properties. Moreover, PAMAM-based carriers increase the possibility of bioavailability of problematic drugs. Hence, PAMAM nanocarriers enhance the potential of the bioavailability of drugs, which are not so soluble for efflux transporters, see [38,39]. Due to these properties, PAMAM dendrimers were extensively studied since their synthesis in 1985, see [40,41]. Donald A. Tomalia brought in the PAMAM (polyamidoamine) as a novel class of polymers, called starburst polymers [40]. From then on, the study of PAMAM dendrimers has remained the most prominent topic of research due to its various applications in different fields, including biomedical applications. For further detail and biomedical application, we refer [42].

Let $D_1(n)$ be the molecular graph of this dendrimers, where n represents the generation stage of $D_1(n)$. The molecular graph of PAMAM dendrimer has four branches, and the central core has four vertices. The total number of vertices in each branch is $13 \times 2^0 + 13 \times 2^1 + \cdots + 13 \times 2^{n-1} + 3 \times 2^n + 5 = 16 \times 2^n - 8$. Hence, the total number of vertices in this molecular graph is $4(16 \times 2^n - 8) + 4 = 64 \times 2^n - 28$. In [43], it is shown that for a given tree graph G (Tree is a connected graph which has no cycle), it follows that $|E(G)| = |V(G)| - 1$. Since PAMAM dendrimer is a tree graph, the total number of edges is $64 \times 2^n - 29$. The chemical structure of this dendrimer is shown in Figure 1.

Theorem 1. *Let $D_1(n)$ be the molecular graph of PAMAM dendrimer, where $n \geq 0$ is the generation. Then the irregularity indices are given by*

$$\begin{aligned} irr(D_1(n)) &= 48 \times 2^n - 22, \\ irr_t(D_1(n)) &= 552 \times 4^n - 476 \times 2^n + 102, \\ \sigma(D_1(n)) &= 64 \times 2^n - 30, \\ Var(D_1(n)) &= \frac{384 \times 4^n - 328 \times 2^n + 69)}{4(16 \times 2^n - 7)^2}. \end{aligned}$$

Proof. The order and size of $D_1(n)$ are $64 \times 2^n - 28$ and $64 \times 2^n - 29$, respectively. Let $V_i^3(n)$ be the set of vertices of degree i in $D_1(n)$. We can classify the vertices of $V(D_1(n))$ into three partite sets, the orders of these sets are $|V_1^3(n)| = 12 \times 2^n - 4$, $|V_2^3(n)| = 40 \times 2^n - 18$ and $|V_3^3(n)| = 12 \times 2^n - 6$.

Now, let $E_{jk}^3(n) \subset E(D_1(n))$ be the set of edges that have end vertices of degrees j and k. We make partition of the edge set $E(D_1(n))$ on the basis of degrees of end vertices of each edge which yields four subsets. The cardinalities of these partite subsets are $|E_{12}^3(n)| = 4 \times 2^n$, $|E_{13}^3(n)| = 8 \times 2^n - 4$, $|E_{22}^3(n)| = 24 \times 2^n - 11$, and $|E_{23}^3(n)| = 28 \times 2^n - 14$.

Followed by the above information and the expressions of irregularity indices manifested in Equations (1)–(4), the explicit formulas of these indices can be obtained in the following way:

$$\begin{aligned} irr(D_1(n)) &= \sum_{uv \in E(D_1(n))} |d_{D_1(n)}(u) - d_{D_1(n)}(v)| \\ &= \left(\sum_{uv \in E_{12}^3(n)} + \sum_{uv \in E_{13}^3(n)} + \sum_{uv \in E_{23}^3(n)} \right) |d_{D_1(n)}(u) - d_{D_1(n)}(v)| \\ &= 48 \times 2^n - 22. \end{aligned}$$

$$\begin{aligned} irr_t(D_1(n)) &= \frac{1}{2} \sum_{u,v \in V(D_1(n))} |d_{D_1(n)}(u) - d_{D_1(n)}(v)| \\ &= \frac{1}{2} \Big((12 \times 2^n - 4)(40 \times 2^n - 18) + (12 \times 2^n - 4)(12 \times 2^n - 6) \\ &+ (12 \times 2^n - 6)(40 \times 2^n - 18) \Big) \\ &= 552 \times 4^n - 476 \times 2^n + 102. \end{aligned}$$

$$\begin{aligned} \sigma(D_1(n)) &= \sum_{uv \in E(D_1(n))} (d_{D_1(n)}(u) - d_{D_1(n)}(v))^2 \\ &= \left(\sum_{uv \in E_{12}^3(n)} + \sum_{uv \in E_{13}^3(n)} + \sum_{uv \in E_{23}^3(n)} \right) (d_{D_1(n)}(u) - d_{D_1(n)}(v))^2 \\ &= 64 \times 2^n - 30. \end{aligned}$$

$$\begin{aligned} Var(D_1(n)) &= \frac{1}{n'} \sum_{v \in V(D_1(n))} d_{D_1(n)}^2(v) - \frac{1}{n'^2} \left(\sum_{v \in V(D_1(n))} d_{D_1(n)}(v) \right)^2 \\ &= \frac{1}{n'} \left(\sum_{v \in V_1^3} d_{D_1(n)}^2(v) + \sum_{v \in V_2^3} d_{D_1(n)}^2(v) + \sum_{v \in V_3^3} d_{D_1(n)}^2(v) \right) \\ &- \frac{1}{n'^2} \left(\sum_{v \in V_1^3} d_{D_1(n)}(v) + \sum_{v \in V_2^3} d_{D_1(n)}(v) + \sum_{v \in V_3^3} d_{D_1(n)}(v) \right)^2 \\ &= \frac{1}{64 \times 2^n - 28} ((1)^2(12 \times 2^n - 4) + (2)^2(40 \times 2^n - 18) \\ &+ (3)^2(12 \times 2^n - 6)) - \frac{1}{(64 \times 2^n - 28)^2} (((1)(12 \times 2^n - 4)) \\ &+ (2)(40 \times 2^n - 18) + (3)(12 \times 2^n - 6))^2. \end{aligned}$$

By means of simple calculations, we derive that

$$Var(D_1(n)) = \frac{384 \times 4^n - 328 \times 2^n + 69)}{4(16 \times 2^n - 7)^2}.$$

□

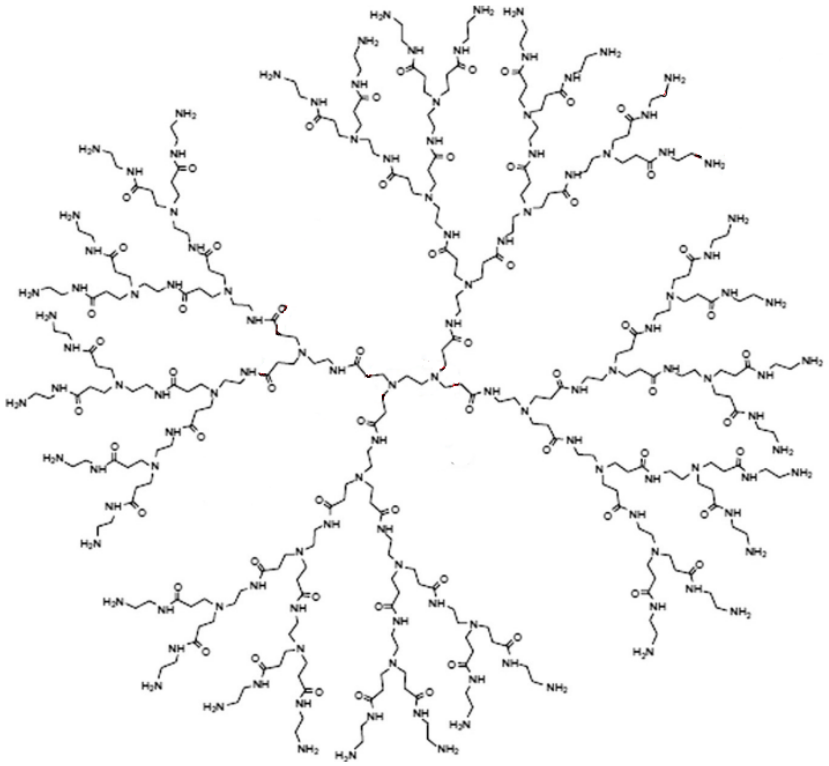

Figure 1. $D_1(n)$ with $n = 3$.

The values of the computed irregularity indices against the different generation stages of PAMAM dendrimers are shown in the Table 1.

Table 1. The values of irregularity indices of structure of Polyamidoamine (PAMAM) dendrimers against different generation stages.

Growth Stage	$irr(D_1(n))$	$irr_t(D_1(n))$	$\sigma(D_1(n))$	$Var(D_1(n))$
$D_1(1)$	74	1358	98	949/2500
$D_1(2)$	170	7030	226	4901/12,996
$D_1(3)$	362	31,622	482	22,021/58,564
$D_1(4)$	746	133,798	994	93,125/248,004
$D_1(5)$	1514	550,118	2018	382,789/1,020,100

The complex synthesis of PAMAM limits the clinical translation of the materials based on PAMAM. Interestingly, PolyEThyleneAmidoAmine (PETAA) dendrimers with more uniform and complete structure then PAMAM possesses several properties of PAMAM. In the next subsection, we will investigate four irregularity indices of PETAA dendrimers.

2.2. Irregularity Measures of PolyEThyleneAmidoAmine (PETAA) Dendrimers

PolyEThyleneAmidoAmine (PETAA) dendrimers have various properties of PAMAM dendrimers such as the number of bonds between the surface, and the dendrimer core is the same. Moreover, the number of surface primary amino groups and tertiary amino groups in PETAA dendrimers are also the same as in PAMAM dendrimers. Other than that, the unique synthesis process of the PETAA enhances its potential for the large-scale production, which results in more application in biomedical sciences [44]. Consequently, the study of PETAA becomes a very respected topic of research. The molecular graph of this dendrimers is denoted by $D_2(n)$, where n represents the generation of $D_2(n)$. The number of vertices in $D_2(n)$ is $44 \times 2^n - 19$ and the number of edges is $44 \times 2^n - 18$. The molecular graph $D_2(n)$ for $n = 5$ is shown in Figure 2.

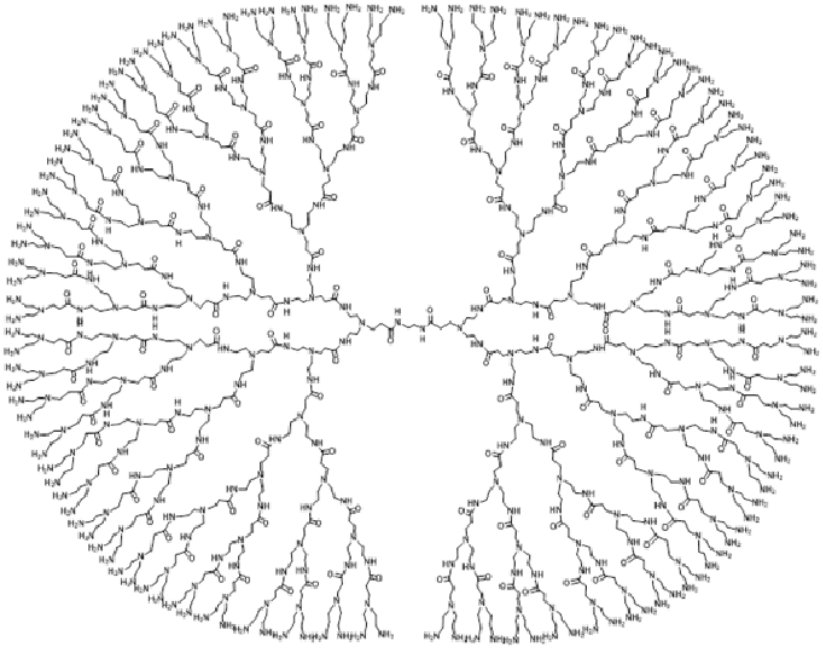

Figure 2. Chemical structure of Poly(EThyleneAmidoAmine) (PETAA) dendrimer $D(5)$.

Theorem 2. *For the molecular graph of PETAA dendrimers $D_2(n)$, the irregularity indices are the following:*

$$\begin{aligned} irr(D_2(n)) &= 32 \times 2^n - 13, \\ irr_t(D_2(n)) &= 256 \times 4^n - 204 \times 2^n + 40, \\ \sigma(D_2(n)) &= 40 \times 2^n - 17, \\ Var(D_2(n)) &= \frac{2(88 \times 4^n - 69 \times 2^n + 13)}{(22 \times 2^n - 9)^2}. \end{aligned}$$

Proof. The order and the size of $D_2(n)$ are $44 \times 2^n - 18$ and $44 \times 2^n - 19$ respectively. Let $V_i^2(n)$ be the set of vertices of degree i in $D_2(n)$. We can classify the vertices of $V(D_2(n))$ into three partite sets; the orders of these sets are $|V_1^2(n)| = 8 \times 2^n - 2$, $|V_2^2(n)| = 28 \times 2^n - 12$, and $|V_3^2(n)| = 8 \times 2^n - 4$.

Now, let $E_{jk}^2(n) \subset E(D_2(n))$ be the set of edges that have end vertices of degrees j and k. There are four types of edges in $E(D_2(n))$ based on the degrees of end vertices of each edge. The cardinalities of these partite sets are $|E_{12}^2(n)| = 4 \times 2^n$, $|E_{13}^2(n)| = 4 \times 2^n - 2$, $|E_{22}^2(n)| = 16 \times 2^n - 8$, and $|E_{23}^2(n)| = 20 \times 2^n - 9$.

Now, with the help of vertex and edge partitions and Equations (1)–(4), the irregularity indices can be computed in the following manner:

$$\begin{aligned} irr(D_2(n)) &= \sum_{uv\in E(D_2(n))} |d_{D_2(n)}(u) - d_{D_2(n)}(v)| \\ &= \left(\sum_{uv\in E^2_{12}(n)} + \sum_{uv\in E^2_{13}(n)} + \sum_{uv\in E^2_{23}(n)} \right) |d_{D_2(n)}(u) - d_{D_2(n)}(v)| \\ &= 32\times 2^n - 13. \end{aligned}$$

$$\begin{aligned} irr_t(D_2(n)) &= \frac{1}{2} \sum_{u,v\in V(D_2(n))} |d_{D_2(n)}(u) - d_{D_2(n)}(v)| \\ &= \frac{1}{2}\Big((8\times 2^n - 2)(28\times 2^n - 12) + (8\times 2^n - 2)(8\times 2^n - 4) \\ &+ (8\times 2^n - 4)(28\times 2^n - 12)\Big) \\ &= 256\times 4^n - 204\times 2^n + 40. \end{aligned}$$

$$\begin{aligned} \sigma(D_2(n)) &= \sum_{uv\in E(D_2(n))} (d_{D_2(n)}(u) - d_{D_2(n)}(v))^2 \\ &= \left(\sum_{uv\in E^2_{12}(n)} + \sum_{uv\in E^2_{13}(n)} + \sum_{uv\in E^2_{23}(n)} \right) (d_{D_2(n)}(u) - d_{D_2(n)}(v))^2 \\ &= 40\times 2^n - 17. \end{aligned}$$

$$\begin{aligned} Var(D_2(n)) &= \frac{1}{n'} \sum_{v\in V(D_2(n))} d^2_{D_2(n)}(v) - \frac{1}{n'^2} \left(\sum_{v\in V(D_2(n))} d_{D_2(n)}(v) \right)^2 \\ &= \frac{1}{n'} \left(\sum_{v\in V^2_1} d^2_{D_2(n)}(v) + \sum_{v\in V^2_2} d^2_{D_2(n)}(v) + \sum_{v\in V^2_3} d^2_{D_2(n)}(v) \right) \\ &- \frac{1}{n'^2} \left(\sum_{v\in V^2_1} d_{D_2(n)}(v) + \sum_{v\in V^2_2} d_{D_2(n)}(v) + \sum_{v\in V^2_3} d_{D_2(n)}(v) \right)^2 \\ &= \frac{1}{44\times 2^n - 18}((1)^2(8\times 2^n - 2) + (2)^2(28\times 2^n - 12) \\ &+ (3)^2(8\times 2^n - 4)) - \frac{1}{(44\times 2^n - 18)^2}(((1)(8\times 2^n - 2)) \\ &+ (2)(28\times 2^n - 12) + (3)(8\times 2^n - 4))^2. \end{aligned}$$

After simplification, we get

$$Var(D_2(n)) = \frac{2(88\times 4^n - 69\times 2^n + 13)}{(22\times 2^n - 9)^2}.$$

□

The Table 2 describes the values of the computed irregularity indices against the different generation stages of PETAA dendrimers.

Table 2. The values of irregularity indices of structure of PETAA dendrimers against different generation stages.

Growth Stage	$irr(D_2(n))$	$irr_t(D_2(n))$	$\sigma(D_2(n))$	$Var(D_2(n))$
$D_2(1)$	51	656	63	454/1225
$D_2(2)$	115	3320	143	2290/6241
$D_2(3)$	243	14,792	303	10,186/27,889
$D_2(4)$	499	62,312	623	42,874/117,649
$D_2(5)$	1011	255,656	1263	175,834/483,025

In 2003, another dendrimer poly (propyl ether imine) (PETIM) was synthesized [45] and reported as a carrier for the sustained delivery of the drug ketoprofen [46]. In the last subsection, we are going to highlight the irregularity-based topological indices of this dendrimers.

2.3. Irregularity Measures of Poly (propyl ether imine) (PETIM) Dendrimers

Zidovudine (AZT) is the first antiretroviral drug approved by the Food and Drug Administration (FDA) for the treatment of Acquired Immune Deficiency Syndrome (AIDS) [47]. In a recent investigation, AZT-loaded PETIM dendrimer for its sustained drug delivery was studied. The findings of the present study revealed that PETIM dendrimer is a better alternative for sustained drug delivery of zidovudine in comparison to present conventional therapy [48]. Let $D_3(n)$ be the molecular graph of this dendrimers, where n represents the generation stage of $D_3(n)$. The molecular graph $D_3(n)$ for $n = 5$ is shown in Figure 3.

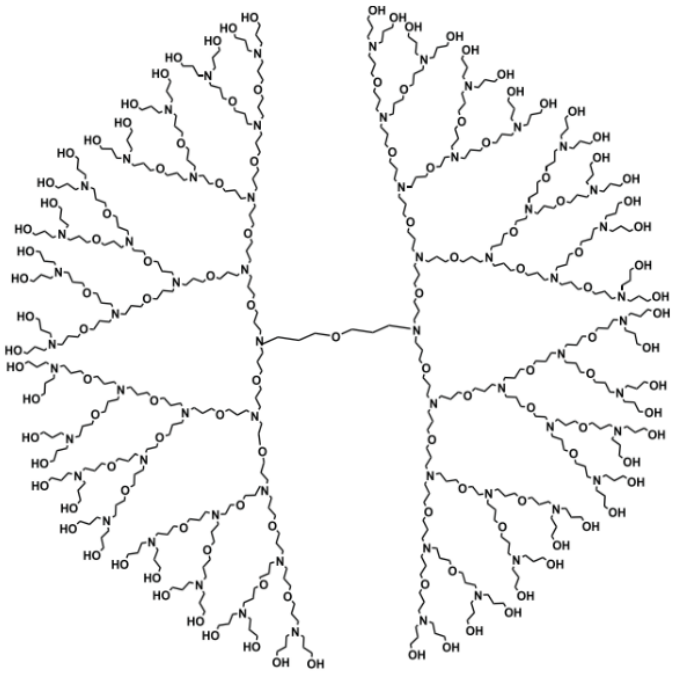

Figure 3. $D_3(n)$ with $n = 5$.

Theorem 3. *For the molecular graph $D_3(n)$, the irregularity indices can be represented by the following formulas:*

$$\begin{aligned} irr(D_3(n)) &= 8\times 2^n - 6 = \sigma(D_3(n)),\\ irr_t(D_3(n)) &= 40\times 4^n - 62\times 2^n + 21,\\ \sigma(D_3(n)) &= 8\times 2^n - 6,\\ Var(D_3(n)) &= \frac{96\times 4^n - 140\times 2^n + 42}{(24\times 2^n - 23)^2}. \end{aligned}$$

Proof. The order and the size of $D_3(n)$ are $3\times 2^{n+3} - 23$ and $24(2^n - 1)$ respectively. Let $V_i^1(n)$ be the set of vertices of degree i in $D_3(n)$. We can classify the vertices of $V(D_3(n))$ into three partite sets, the orders of these sets are $|V_1^1(n)| = 2^{n+1}$, $|V_2^1(n)| = 5\times 2^{n+2} - 21$, and $|V_3^1(n)| = 2^{n+1} - 2$.

Now, let $E_{jk}^1(n) \subset E(D_3(n))$ be the set of edges that have end vertices of degrees j and k. There are three types of edges in $E(D_3(n))$ based on the degrees of end vertices of each edge. The cardinalities of these partite sets are $|E_{12}^1(n)| = 2^{n+1}$, $|E_{22}^1(n)| = 2(2\times 2^{n+3} - 9)$, and $|E_{23}^1(n)| = 6(2^n - 1)$.

Followed by the above information, and the expressions of irregularity indices manifested in Equations (1)–(4), the explicit formulae of these indices can be formulated as follows:

$$\begin{aligned} irr(D_3(n)) &= \sum_{uv\in E(D_3(n))} |d_{D_3(n)}(u) - d_{D_3(n)}(v)|\\ &= \left(\sum_{uv\in E_{12}^1(n)} + \sum_{uv\in E_{23}^1(n)}\right) |d_{D_3(n)}(u) - d_{D_3(n)}(v)|\\ &= 8\times 2^n - 6. \end{aligned}$$

$$\begin{aligned} irr_t(D_3(n)) &= \frac{1}{2}\sum_{u,v\in V(D_3(n))} |d_{D_3(n)}(u) - d_{D_3(n)}(v)|\\ &= \frac{1}{2}\Big((2^{n+1})(5\times 2^{n+2} - 21) + (5\times 2^{n+2} - 21)(2^{n+1} - 2)\Big)\\ &= 40\times 4^n - 62\times 2^n + 21. \end{aligned}$$

$$\begin{aligned} \sigma(D_3(n)) &= \sum_{uv\in E(D_3(n))} (d_{D_3(n)}(u) - d_{D_3(n)}(v))^2\\ &= \left(\sum_{uv\in E_{12}^1(n)} + \sum_{uv\in E_{23}^1(n)}\right) (d_{D_3(n)}(u) - d_{D_3(n)}(v))^2\\ &= 8\times 2^n - 6. \end{aligned}$$

$$
\begin{aligned}
Var(D_3(n)) &= \frac{1}{n'}\sum_{v\in V(D_3(n))} d^2_{D_3(n)}(v) - \frac{1}{n'^2}\left(\sum_{v\in V(D_3(n))} d_{D_3(n)}(v)\right)^2 \\
&= \frac{1}{n'}\left(\sum_{v\in V_1^1} d^2_{D_3(n)}(v) + \sum_{v\in V_2^1} d^2_{D_3(n)}(v) + \sum_{v\in V_3^1} d^2_{D_3(n)}(v)\right) \\
&- \frac{1}{n'^2}\left(\sum_{v\in V_1^1} d_{D_3(n)}(v) + \sum_{v\in V_2^1} d_{D_3(n)}(v) + \sum_{v\in V_3^1} d_{D_3(n)}(v)\right)^2 \\
&= \frac{1}{3\times 2^{n+3}-23}((1)^2(2^{n+1}) + (2)^2(5\times 2^{n+2}-21) \\
&+ (3)^2(2^{n+1}-2)) - \frac{1}{(3\times 2^{n+3}-23)^2}(((1)(2^{n+1})) \\
&+ (2)(5\times 2^{n+2}-21) + (3)(2^{n+1}-2))^2.
\end{aligned}
$$

Further simplifications yield

$$
Var(D_3(n)) = \frac{96\times 4^n - 140\times 2^n + 42}{(24\times 2^n - 23)^2}.
$$

□

The Table 3 presents the values of the computed irregularity indices against the different generation stages of PETIM dendrimers. In the next section, we present some graphical analysis of irregularity measures (of the structures under discussion) based upon the results obtained in this section.

Table 3. The values of irregularity indices of structure of poly (propyl ether imine) (PETIM) dendrimers against different generation stages.

Growth Stage	$irr(D_3(n))$	$irr_t(D_3(n))$	$\sigma(D_3(n))$	$Var(D_3(n))$
$D_3(1)$	10	57	10	146/625
$D_3(2)$	26	413	26	1018/5329
$D_3(3)$	58	2085	58	5066/28,561
$D_3(4)$	122	9269	122	22,378/130,321
$D_3(5)$	250	38,997	250	93,866/55,5025

3. Graphical Analysis and Discussions

In this section, we present our theoretical outcomes and deduce which of the dendrimer structures depicted above is more irregular than the remaining ones with respect to a specific irregularity index. Each dendrimer structure relies on a single variable n. We plot the graph with irregularity index of $D_1(n)$, $D_2(n)$, and $D_3(n)$ (on a single graph) as a dependent variable and n as an independent variable. We observe that all the irregularity indices behave in a particular way with the increase in the value of n. We provided the graphical appearances of these indices with respect to the change in the growth stage of the dendrimer structure. In this graphical examination, the blue colour shows the graphical functioning of the PETIM dendrimer structure, the red colour shows the graphical behaviour of the PETAA dendrimer structure, and the green colour shows the graphical response of the PAMAM dendrimer structure. We present the values of various irregularity indices for the dendrimer structures in Tables 1–3. With the help of these tables, the comparative behavior of these irregularity indices for dendrimer structures has been expressed in Figures 4–7. These figures show that the molecular structure of PAMAM dendrimer is highly irregular as compared to the other dendrimer structures

and the molecular structure of PETAA dendrimer is more irregular than the molecular structure of PETIM dendrimer.

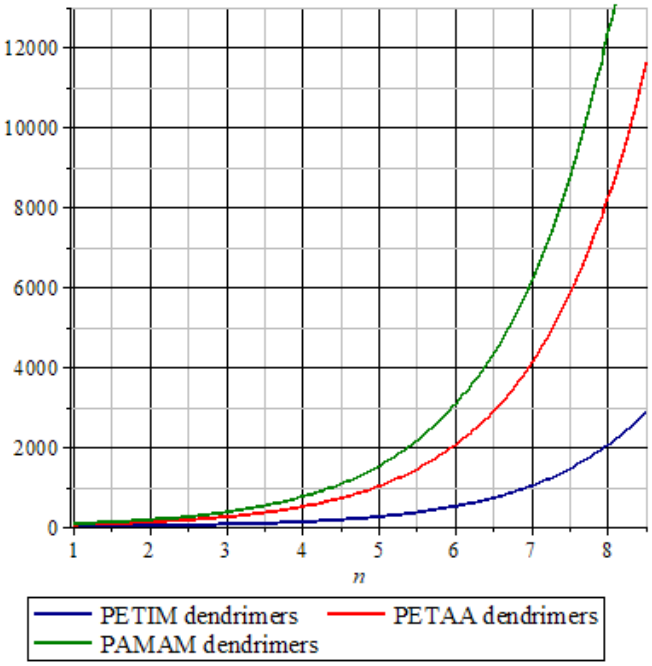

Figure 4. Albertson irregularity index.

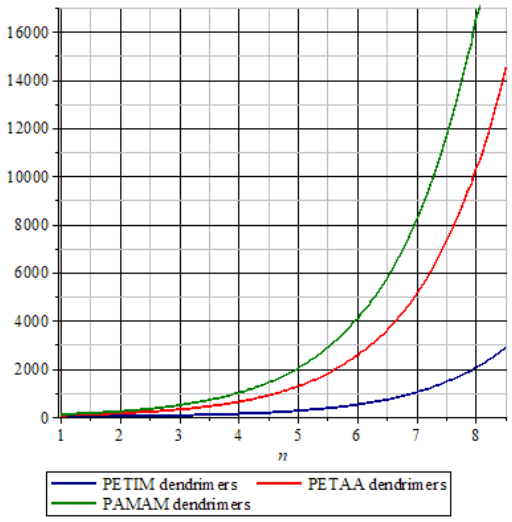

Figure 5. σ irregularity index.

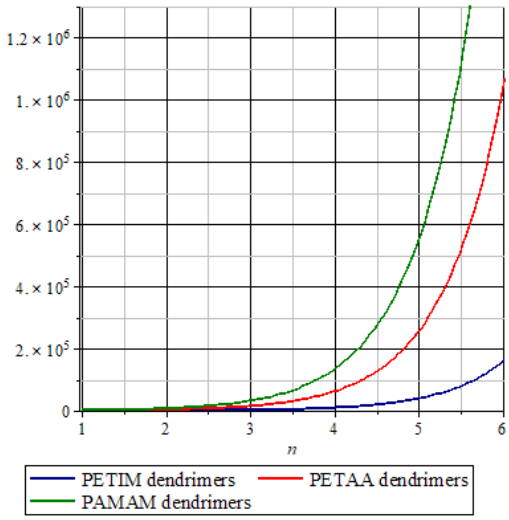

Figure 6. Total irregularity index.

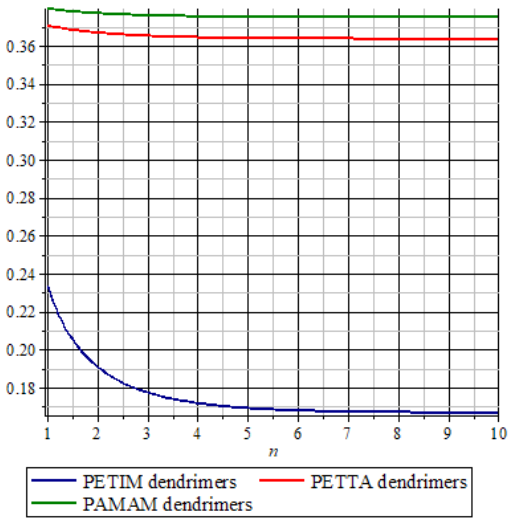

Figure 7. Variance index.

4. Conclusions

A modern trend in QSAR/QSPR studies is the use of properties which can be secure from the molecular structure without any other input data. The basic reason for this is to forecast the chemical properties of such a huge collection of compounds and drugs takes a large number of chemical inspections, thereby these tasks increase the burden of work of the chemical and pharmaceutical researchers. Thus, the strategy of estimating the topological indices has offered the explanations of such medicinal behaviour of various compounds and drugs. Hence, the irregularity indices for the molecular graphs of dendrimers are demonstrated by a mathematical derivation method and we presented the comparison of the molecular structures by using the graph structures. Our outcomes could perform a significant role in estimating and comparing the properties of these molecular structures.

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