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Research Article

Computing SS Index of Certain Dendrimers

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The numerical descriptor gathers the data from the molecular graphs and helps to know the characteristics of the chemical structure known as topological index. The QSAR/QSPR/QSTR studies are benefited with the significant role played by topological indices in the drug design. Topological indices provide the information about the physical/chemical/biological properties of chemical compounds. The Zagreb indices are widely studied because of their extensive usage in chemical graph theory. Inspired by the earlier work on inverse sum indeg index (ISI index), novel topological index known as SS index is introduced and computed for four dendrimer structures. Also, the strong correlation coefficient between SS index and 5 physico-chemical characteristics such as boiling point (*bp*), molar volume (*mv*), molar refraction (*mr*), heats of vaporization (*hv*), and critical pressure (*cp*) of 67 alkane isomers have been determined. It is found that newly introduced index has shown good correlation in comparison with three most popular existing indices (ISI index and first and second Zagreb indices). In the last part, the mathematical properties of SS index are discussed.

1. Introduction and Terminologies

Every year, large number of new drugs are produced due to the rapid growth of medicine manufacturing. As a result, determining the pharmacological, chemical, and biological characteristics of a substance necessitates a significant amount of effort.

These new medications are becoming increasingly clumsy and clumped. In order to check the performance of new drugs and their side effects, sufficient reagents, equipment, and technicians are needed. However, in low-income countries, there is an insufficient funding to cover the costs of reagents and equipment needed to calculate biochemical properties. The existing studies have shown that the chemical and pharmacodynamic properties of drugs, as well as their molecular structures, are inextricably related. If we quantify measures of these drug molecular structures with the aim of identifying topological indices, medical and pharmaceutical researchers will be able to understand their therapeutic properties, which can compensate for the shortcomings of medicine and chemical experiments. In this regard, the methods computing topological index are suitable and useful for developing countries, as they can produce accessible biological and medical knowledge about new drugs without the use of chemical experiment hardware. To calculate the characteristics of drug molecules, the PI index, Zagreb index, and eccentric index are used. The number of vertices and edges of a chemical compound counts to the computation of topological indices [1–8].

A topological index is a computational parameter derived from the graph structure mathematically [9–13]. To visualize the relationships between the data sets, graphs are crucial tools which make the concept better understandable. A descriptor that gives the data regarding arrangement of

atoms in a compound in numerical form of information regarding its shape, branching, and other data of a compound is a topological index.

The significant number of early drug studies suggests that the biomedical and pharmacology properties of drugs, as well as their molecular structures, have a clear inner relationship. Many scientists have developed various indices to quantify the characteristics of drug molecules over the last 40 years. The indices are of great use in the study of pharmacology, toxicology, and chemistry (QSAR/QSPR/QSTR) [14–16].

Dendrimers are also called "cascade molecules," but this term is not in general use compared to the term dendrimers. In 1978, Fritz Vogtle was the first to bring these nanomolecules into light. Dendrites normally include a unique chemically addressable unit known as focus or core. The usage and popularity of dendrimers have been greatly increased. Since 2005, there have been over 5000 research papers and patents. A second group of the synthesized macromolecules is called arborols. We can say that the molecules of dendrimers are of architectural design. These thoroughly tailored architectural nanomolecules can be functionalized and modify their physico-chemical or biological characteristics.

The hyper-branched macromolecules have three phases in its structural constitution. An atom at the centre of the structure called the core of the dendrimer has some functional properties. Secondly, the branches are ejected out of the core and add on the branches repetitively. Finally, the terminal groups are situated on the surface of the dendritic structure. Dendrimer synthesis is divided into two methods: divergent synthesis and convergent synthesis. It is difficult to synthesize dendrimers using either approach, because the actual reactions require several steps to protect the active site. As a result, it is difficult to manufacture and prohibitively costly to buy. Dendrites have significant applications in biomedical field because of its characteristics, including hyper-branching, well-defined globular structures, outstanding structural uniformity, multivalency, varying chemical constitution, and higher biological compatibility.

In medical field, mathematical modelling is used to analyse the representation of emerging drugs, normally as an undirected graph, such that each vertex depicts an atom and an edge depicts a link between atoms. Every year new drugs are available and needs remarkable work to select the qualities of the emerging drugs. Dendrimers are a good option in the drug design because of its biological characteristics such as polyvalency, self-assembling, electrostatic interactions, chemical stability, low cytotoxicity, and solubility. The remarkable and emerging role of dendritic macromolecules is in therapies of anticancer and image diagnosis.

Various studies have revealed that there is a consistent correlation between the molecular structures of compounds, drugs, and their characteristics. Topological indices are numerical variants that assist researchers in understanding physical properties, chemical interactions, and biological activity [17–21]. Hence, the discussion on topological indices of chemical structures of drugs helps to know the theoretical basis to prepare new drugs. In this study, SS index is defined and computed for porphyrin (D_nP_n), propyl ether imine (DPZ_n), zinc porphyrin (PETIM), and polyethylene amide amine (PETAA) dendrimers [22,23].

In this paper, the notations and terminologies pertaining to the graphs are found in [24].

Definition 1. The oldest and the most studied indices, the first and second Zagreb indices [25], proposed by Gutman and Trinajstić are defined as

$$M_1(G) = \sum_{v\omega \epsilon E(G)} (d_v + d_\omega),$$
$$M_2(G) = \sum_{v\omega \epsilon E(G)} (d_v . d_\omega). \quad (1)$$

Definition 2. Vukičević et al. introduced inverse sum indeg index [26] and stated as

$$\mathrm{ISI}(G) = \sum_{v\omega \in E(G)} \frac{d_v . d_\omega}{d_v + d_\omega}. \quad (2)$$

Definition 3. In this work, a novel invariant known as SS (Shilpa-Shanmukha) index is introduced and studied. This index is defined as follows:

$$\mathrm{SS}(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_v . d_\omega}{d_v + d_\omega}}. \quad (3)$$

Throughout this article, d_v and d_ω represent the degrees of vertices v and ω, respectively.

2. Chemical Applicability of the SS Index through QSPR Analysis

Here, we discussed the proposed topological index known as SS index to study the physico-chemical properties, namely, *bp, mv, mr, hv,* and *cp* of 67 alkanes ranging from *n*-butanes to nonanes. The 5 physico-chemical properties of 67 alkane isomers can be found in [27] and Table 1 represents the computed values of four topological indices (SS, ISI, M_1, and M_2) of 67 alkane isomers. The 5 characteristics of alkane isomers are correlated with SS index and it is found that SS index has shown good correlation with all the 5 properties compared to the existing three most popular indices M_1, M_2, and ISI considered in the study. The SS index is plotted against each of the 5 properties of alkane isomers which is depicted in Figure 1.

Regression model for properties of alkane isomers.

The linear regression model is given by

$$P = m(\mathrm{TI}) + c, \quad (4)$$

where P is the physical property and TI is the topological index. Equation (4) results in the following linear regression models for various properties with SS index.

Table 1: The values of various topological indices of alkanes.

SI. No.	Alkane	SS (G)	ISI (G)	M_1 (G)	M_2 (G)
1	Butane	2.8165	2.6667	10	8
2	2-Methyl propane	2.598	2.25	12	4
3	Pentane	2.9428	3.3333	14	12
4	2-Methyl butane	3.644	3.3667	16	14
5	2,2-Dimethyl propane	3.5777	3.2	20	16
6	Hexane	4.633	4.3333	18	16
7	2-Methyl pentane	4.644	4.3667	20	18
8	3-Methyl pentane	4.69	4.4833	20	19
9	2,2-Methyl butane	4.6545	4.4	24	22
10	2,3-Dimethyl butane	4.6888	4.5	22	21
11	Heptane	5.633	5.3333	22	20
12	2-Methyl hexane	5.644	5.3667	24	22
13	3-Methyl hexane	5.6899	5.4833	24	23
14	3-Ethyl pentane	5.7358	5.6	24	24
15	2,2-Dimethyl pentane	5.6544	5.4	28	26
16	2,3-Dimethyl pentane	5.7347	5.616	26	26
17	2,4-Dimethyl pentane	5.655	5.4	26	24
18	3,3-Dimethyl pentane	5.7312	5.6	28	28
19	Octane	6.633	6.333	26	24
20	2-Methyl heptane	6.644	6.3667	28	26
21	3-Methyl heptane	6.69	6.4833	28	27
22	4-Methyl heptane	6.68	6.49	28	27
23	3-Ethyl hexane	6.736	6.6	28	28
24	2,2-Dimethyl hexane	6.6545	6.4	32	30
25	2,3-Dimethyl hexane	6.7348	6.6166	30	30
26	2,4-Dimethyl hexane	6.7009	6.5166	30	29
27	2,5-Dimethyl hexane	6.655	6.4	32	30
28	3,3-Dimethyl hexane	6.7312	6.6	32	32
29	3,4-Dimethyl hexane	6.7807	6.7333	30	31
30	3-Ethyl-2-methyl pentane	6.7807	6.7333	30	22
31	3-Ethyl-3-methyl pentane	6.808	6.8	32	34
32	2,2,3-Trimethyl pentane	6.7706	6.731	34	35
33	2,2,4-Trimethyl pentane	6.6655	6.4333	34	32
34	2,3,3-Trimethyl pentane	6.8014	6.8143	34	36
35	2,3,4-Trimethyl pentane	6.7796	6.75	32	33
36	Nonane	7.6333	7.3333	30	28
37	2-Methyl octane	7.644	7.3667	32	30
38	3-Methyl octane	7.69	7.4833	32	31
39	4-Methyl octane	7.69	7.4833	32	31
40	3-Ethyl heptane	7.7358	7.6	32	32
41	4-Ethyl heptane	7.7358	7.6	32	32
42	2,2-Dimethyl heptane	7.6545	7.4	36	34
43	2,3-Dimethyl heptane	7.7348	7.6166	34	34
44	2,4-Dimethyl heptane	7.7009	7.5166	34	33
45	2,5-Dimethyl heptane	7.7963	7.7166	34	33
46	2,6-Dimethyl heptane	7.655	7.4	34	32
47	3,3-Dimethyl heptane	7.7312	7.6	36	36
48	3,4-Dimethyl heptane	7.7807	7.7333	34	35
49	3,5-Dimethyl heptane	7.7468	7.6333	34	34
50	4,4-Dimethyl heptane	7.7312	7.6	36	36
51	3-Ethyl-2-methyl hexane	7.7807	7.7333	34	35
52	4-Ethyl-2-methyl hexane	7.9246	8.0333	34	34
53	3-Ethyl-3-methyl hexane	7.808	7.8	36	36
54	2,2,4-Trimethyl hexane	7.7114	7.55	38	37
55	2,2,5-Trimethyl hexane	7.6655	7.4333	38	36
56	2,3,3-Trimethyl hexane	7.8014	7.8143	38	40
57	2,3,4-Trimethyl hexane	7.8255	7.8667	36	44
58	2,3,5-Trimethyl hexane	7.7458	7.65	36	44
59	3,3,4-Trimethyl hexane	7.8845	8	38	41
60	3,3-Diethyl pentane	7.866	7.931	44	40

Table 1: Continued.

SI. No.	Alkane	SS (G)	ISI (G)	M_1 (G)	M_2 (G)
61	2,2-Dimethyl-3-ethyl pentane	7.878	8.0143	54	40
62	2,3-Dimethyl-3-ethyl pentane	7.8255	7.8666	46	42
63	2,4-Dimethyl-3-ethyl pentane	7.8575	8	44	38
64	2,2,3,3-Tetramethyl pentane	7.8575	8	42	46
65	2,2,3,4-Tetramethyl pentane	7.8154	7.643	40	42
66	2,2,4,4-Tetramethyl pentane	7.676	7.4667	42	40
67	2,3,3,4-Tetramethyl pentane	7.8715	8.0281	40	44

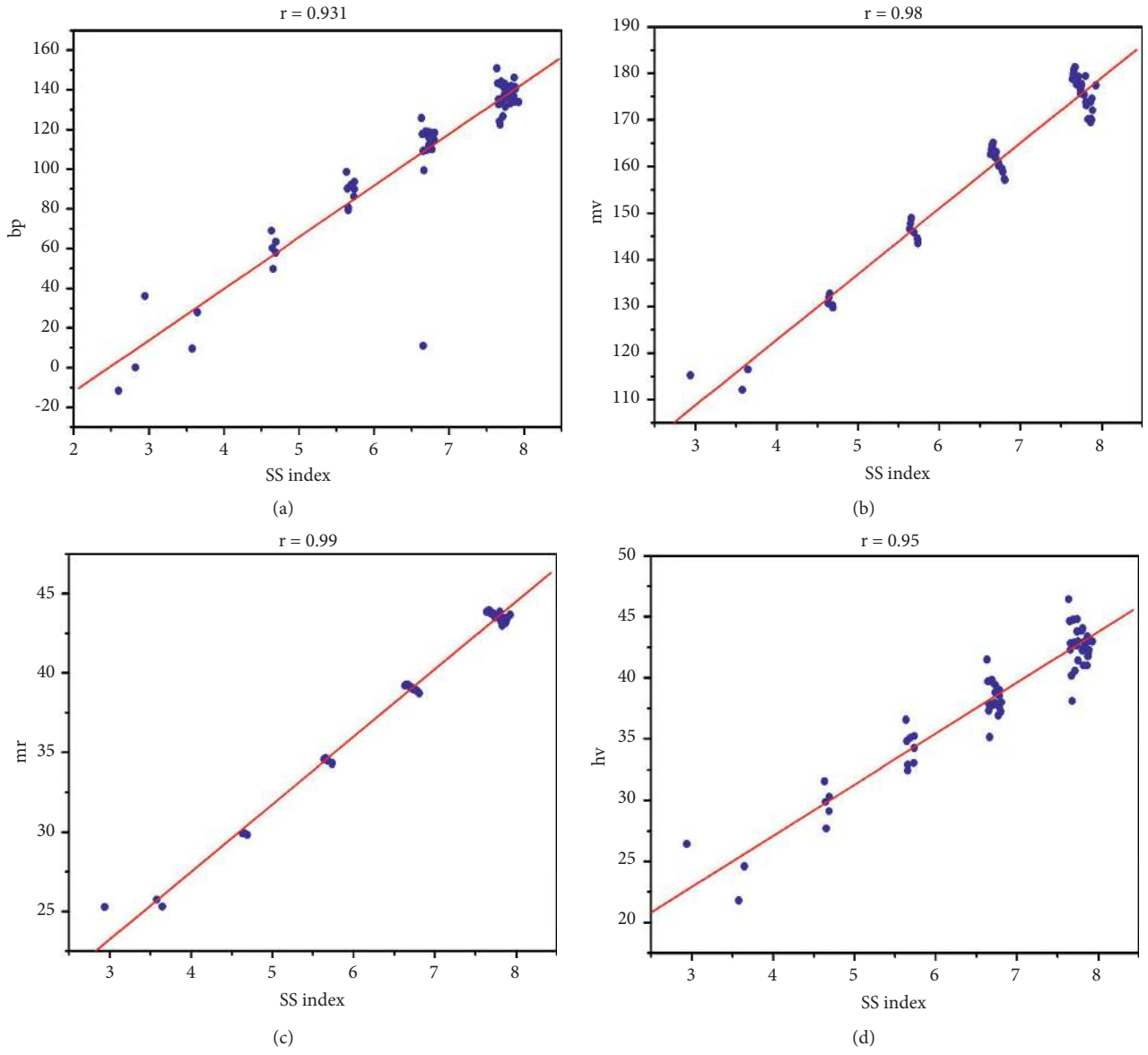
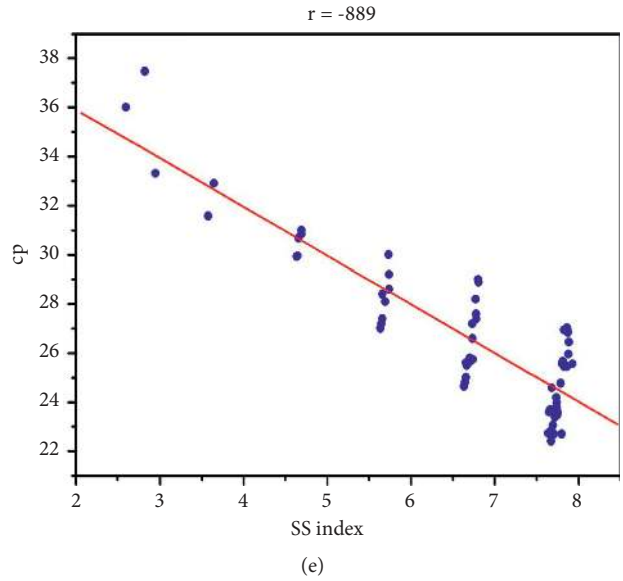


Figure 1: Continued.



(e)

Figure 1: Correlation of SS index with properties of alkane isomers.

$$\begin{aligned} bp &= -64.28 + 25.99\,(\mathrm{SS}),\\ mv &= 66.57 + 14.07\,(\mathrm{SS}),\\ mr &= 10.46 + 4.26\,(\mathrm{SS}),\\ hv &= 10.4 + 4.173\,(\mathrm{SS}),\\ cp &= 39.87 - 1.98\,(\mathrm{SS}). \end{aligned} \tag{5}$$

The SS index has correlation coefficients of 0.931, 0.98, 0.99, 0.951, and –0.889 with residual standard errors 14.46, 3.76, 0.57, 1.69, and 1.45 and all these models are statistically significant, since the level of significance value of all models is less than 0.05.

Some important observations from the data are presented in Table 2. The correlation coefficients of *bp*, *mv*, *mr*, and *hv* have shown high positive correlation for the introduced SS index. Also, it is interesting to know that the correlation coefficient for *cp* shows highly negative correlation for the SS index.

Table 2: The correlation coefficient between SS, ISI, M_1, and M_2 indices with some physico-chemical properties of alkane isomers.

Properties	*bp*	*mv*	*mr*	*hv*	*cp*
SS (G)	0.931	0.98	0.99	0.951	−0.889
ISI (G)	0.931	0.96	0.984	0.942	−0.855
M_1 (G)	0.779	0.799	0.837	0.715	−0.684
M_2 (G)	0.816	0.8065	0.854	0.737	−0.688

3. Dendrimers

Dendrimers, come from the Greek word which means "trees," are branched at the core and they form a spherical three-dimensional structure. Dendrimers have attracted a lot of researchers globally in the study of topological indices [28–33]. The aim of this paper is to compute SS index of four dendrimer structures, namely, D_nP_n, DPZ_n, PETIM, and PETAA.

3.1. SS Index of Porphyrin Dendrimer (D_nP_n). Consider the porphyrin dendrimer family. This family of dendrimers is denoted by D_nP_n. The molecular graph of D_nP_n is shown in Figure 2.

Let G be the molecular graph of D_nP_n. By calculation, it is found that G consists of number of vertices and edges to be $96n - 10$ and $105n - 11$, respectively. Table 3 shows the six forms of edges in $D_nP_n(G)$ based on degrees of end vertices of each edge.

Theorem 1. *Let D_nP_n be the family of porphyrin dendrimers. Then, the SS index of D_nP_n is given by*

$$\mathrm{SS}(D_nP_n) = \left[2\left(\frac{3}{4}\right)^{1/2} + 24\left(\frac{4}{5}\right)^{1/2} + 10 + 48\left(\frac{6}{5}\right)^{1/2} + 13\left(\frac{9}{6}\right)^{1/2} + 8\left(\frac{12}{7}\right)^{1/2}\right]n - \left[5 + 6\left(\frac{6}{5}\right)^{1/2}\right]. \tag{6}$$

Proof. From the definition of SS index and Table 3, we deduce

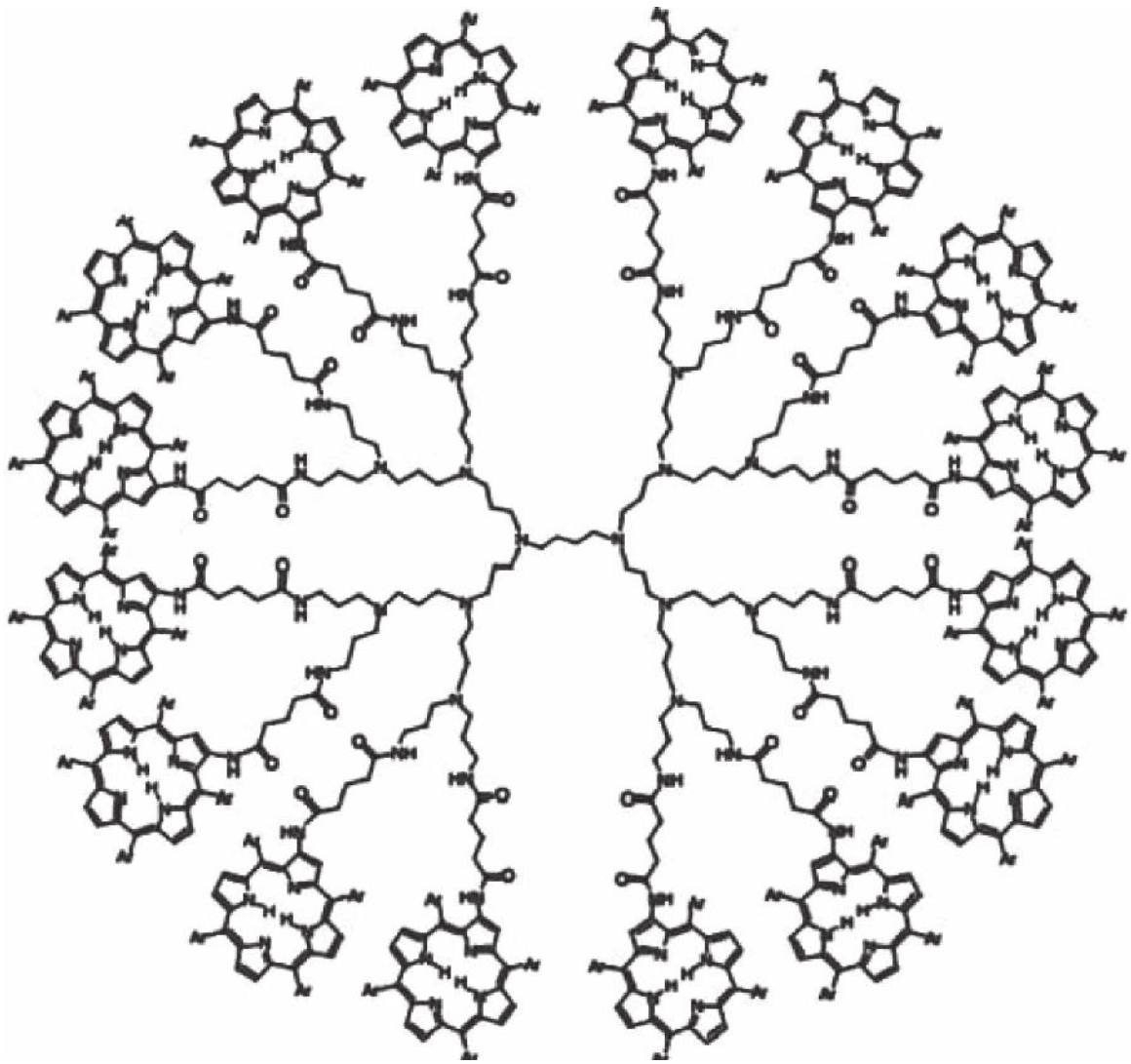


Figure 2: The molecular graph of porphyrin dendrimer.

Table 3: Edge partition of D_nP_n.

(d_ν, d_ω), where $\nu\omega \in E(G)$	$(1,3)$	$(1,4)$	$(2,2)$	$(2,3)$	$(3,3)$	$(3,4)$
Number of edges	$2n$	$24n$	$10n-5$	$48n-6$	$13n$	$8n$

$$\begin{aligned} SS(D_nP_n) &= \sum_{\nu\omega\in E(G)} \sqrt{\frac{d_\nu d_\omega}{d_\nu + d_\omega}} = 2n\left(\frac{1\times 3}{1+3}\right)^{1/2} + 24n\left(\frac{1\times 4}{1+4}\right)^{1/2} + (10n-5)\left(\frac{2\times 2}{2+2}\right)^{1/2} + (48n-6)\left(\frac{2\times 3}{2+3}\right)^{1/2} \\ &\quad + 13n\left(\frac{3\times 3}{3+3}\right)^{1/2} + 8n\left(\frac{3\times 4}{3+4}\right)^{1/2}, \\ SS(D_nP_n) &= \left[2\left(\frac{3}{4}\right)^{1/2} + 24\left(\frac{4}{5}\right)^{1/2} + 10 + 48\left(\frac{6}{5}\right)^{1/2} + 13\left(\frac{9}{6}\right)^{1/2} + 8\left(\frac{12}{7}\right)^{1/2}\right]n - \left[5 + 6\left(\frac{6}{5}\right)^{1/2}\right]. \end{aligned} \tag{7}$$

□

3.2. SS Index of Zinc Porphyrin Dendrimer (DPZ_n). Consider the zinc porphyrin dendrimer family. This family of dendrimers is represented by DPZ_n. The molecular graph of DPZ_n is depicted in Figure 3.

Let G be the molecular graph of DPZ_n. By calculation, it is found that G has $56 \times 2^n - 7$ vertices and $64 \times 2^n - 4$ edges. Table 4 shows the four forms of edges in DPZ_n based on degrees of end vertices of each edge.

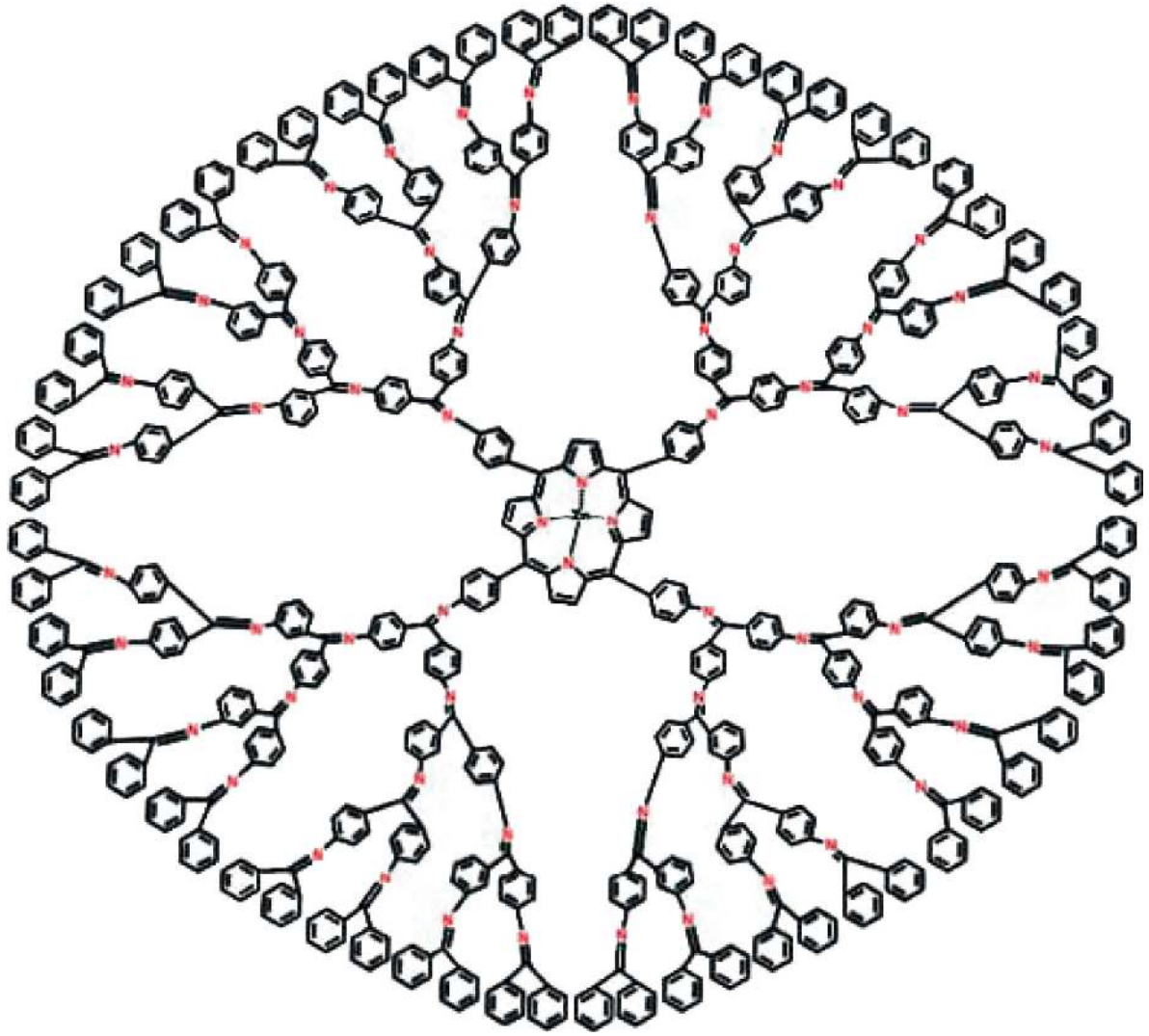


Figure 3: The molecular graph of zinc porphyrin dendrimer.

Table 4: Edge partition of DPZ_n.

(d_v, d_ω), where $v\omega \in E(G)$	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$16 \times 2^n - 4$	$40 \times 2^n - 16$	$8 \times 2^n - 16$	4

Theorem 2. *Let DPZ_n be the family of zinc porphyrin dendrimers. Then, the SS index of DPZ_n is given by*

$$SS(DPZ_n) = \left[16 + 40\left(\frac{6}{5}\right)^{1/2} + 8\left(\frac{9}{6}\right)^{1/2}\right]2^n - \left[4 + 16\left(\frac{16}{5}\right)^{1/2} + 16\left(\frac{9}{6}\right)^{1/2} - 4\left(\frac{12}{7}\right)^{1/2}\right]. \quad (8)$$

Proof. From the definition of SS index and Table 4, we deduce

$$SS(DPZ_n) = \sum_{\nu\omega \in E(G)} \sqrt{\frac{d_\nu d_\omega}{d_\nu + d_\omega}} = (16 \times 2^n - 4)\left(\frac{2\times 2}{2+2}\right)^{1/2} + (40 \times 2^n - 16)\left(\frac{2\times 3}{2+3}\right)^{1/2} + (8 \times 2^n - 16)\left(\frac{3\times 3}{3+3}\right)^{1/2} + 4\left(\frac{3\times 4}{3+4}\right)^{1/2}, \tag{9}$$

$$SS(DPZ_n) = \left[16 + 40\left(\frac{6}{5}\right)^{1/2} + 8\left(\frac{9}{6}\right)^{1/2}\right]2^n - \left[4 + 16\left(\frac{16}{5}\right)^{1/2} + 16\left(\frac{9}{6}\right)^{1/2} - 4\left(\frac{12}{7}\right)^{1/2}\right].$$

□

3.3. SS Index of Propyl Ether Imine Dendrimer (PETIM). Consider the family of propyl ether imine dendrimers. This family of dendrimers is represented by PETIM. The molecular graph of PETIM is depicted in Figure 4.

Let G be the molecular graph of PETIM. By calculation, G has $24 \times 2^n - 23$ vertices and $24 \times 2^n - 24$ edges. Table 5 shows the three forms of edges in PETIM based on degrees of end vertices of each edge.

Theorem 3. *Let PETIM be the family of propyl ether imine dendrimers. Then, the SS index of PETIM is given by*

$$SS(PETIM) = \left[2\left(\frac{2}{3}\right)^{1/2} + 16 + 6\left(\frac{6}{5}\right)^{1/2}\right]2^n - \left[18 + 6\left(\frac{6}{5}\right)^{1/2}\right]. \tag{10}$$

Proof. From the definition of SS index and Table 5, we deduce

$$SS(PETIM) = \sum_{\nu\omega \in E(G)} \sqrt{\frac{d_\nu d_\omega}{d_\nu + d_\omega}} = (2 \times 2^n)\left(\frac{1\times 2}{1+2}\right)^{1/2} + (16 \times 2^n - 18)\left(\frac{2\times 2}{2+2}\right)^{1/2} + (6 \times 2^n - 6)\left(\frac{2\times 3}{2+3}\right)^{1/2}, \tag{11}$$

$$SS(PETIM) = \left[2\left(\frac{2}{3}\right)^{1/2} + 16 + 6\left(\frac{6}{5}\right)^{1/2}\right]2^n - \left[18 + 6\left(\frac{6}{5}\right)^{1/2}\right].$$

□

3.4. SS Index of Polyethylene Amide Amine (PETAA) Dendrimer. Consider the family of polyethylene amide amine dendrimers. This family of dendrimers is represented by PETAA. The molecular graph of PETAA is depicted in Figure 5.

Let G be the molecular graph of PETAA. By calculation, G has $44 \times 2^n - 18$ vertices and $44 \times 2^n - 19$ edges. Table 6 shows the four forms of edges in PETAA based on degrees of end vertices of each edge.

Theorem 4. *Let PETAA be the family of zinc porphyrin dendrimers. Then, the SS index of PETAA is given by*

$$SS(PETAA) = \left[4\left(\frac{2}{3}\right)^{1/2} + 4\left(\frac{3}{4}\right)^{1/2} + 16 + 20\left(\frac{6}{5}\right)^{1/2}\right]2^n - \left[2\left(\frac{3}{4}\right)^{1/2} + 8 + 9\left(\frac{6}{5}\right)^{1/2}\right]. \tag{12}$$

Proof. From the definition of SS index and Table 6, we deduce

$$SS(PETAA) = \sum_{\nu\omega \in E(G)} \sqrt{\frac{d_\nu d_\omega}{d_\nu + d_\omega}} = (4 \times 2^n)\left(\frac{1\times 2}{1+2}\right)^{1/2} + (4 \times 2^n - 2)\left(\frac{1\times 3}{1+3}\right)^{1/2} + (16 \times 2^n - 8)\left(\frac{2\times 2}{2+2}\right)^{1/2} + (20 \times 2^n - 9)\left(\frac{2\times 3}{2+3}\right)^{1/2}, \tag{13}$$

$$SS(PETAA) = \left[4\left(\frac{2}{3}\right)^{1/2} + 4\left(\frac{3}{4}\right)^{1/2} + 16 + 20\left(\frac{6}{5}\right)^{1/2}\right]2^n - \left[2\left(\frac{3}{4}\right)^{1/2} + 8 + 9\left(\frac{6}{5}\right)^{1/2}\right].$$

□

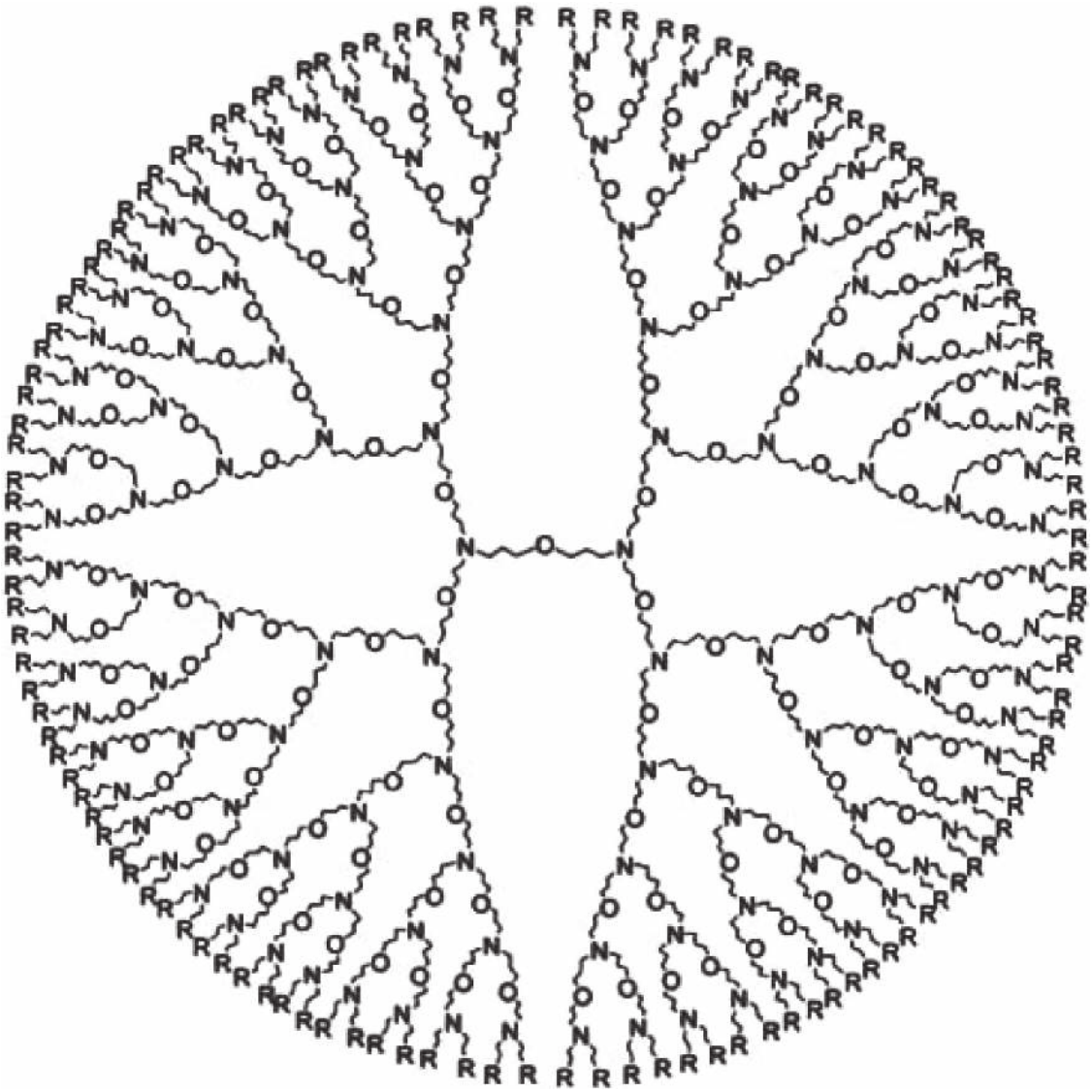


Figure 4: The molecular graph of propyl ether imine dendrimer.

Table 5: Edge partition of PETIM.

(d_v, d_ω), where $v\omega \in E(G)$	$(1,2)$	$(2,2)$	$(2,3)$
Number of edges	2×2^n	$16 \times 2^n - 18$	$6 \times 2^n - 6$

4. Results and Discussion

In this work, novel topological index known as SS index is introduced and the proposed index is computed for 67 alkane isomers to study the physico-chemical properties, namely, *bp*, *mv*, *mr*, *hv*, and *cp*. A linear regression model of these physical properties with SS index is presented. From Table 2 and Figure 1, the SS index has highest correlation with molar refraction (*mr*) which is 0.99. Also, SS index is with boiling point (*bp*) 0.931, with molar volume (*mv*) 0.98, with heat of vaporization (*hv*) 0.951, and with critical pressure (*cp*) −0.889. From Table 2 by inspection, it is clear that SS index has good correlation with the physico-chemical properties compared to the existing indices, namely, inverse sum indeg index, first Zagreb index, and second Zagreb index. Also, the work focuses on computing the SS index for four dendrimer structures, namely, D_nP_n, DPZ_n, PETIM, and PETAA. The values of n are substituted for $n = 1$ to 10. By inspection from Table 7, it is very clear that SS index increases as n increases. Also, it is observed that correlation coefficient of D_nP_n is $r = 1$, which is more than the correlation coefficients of DPZ_n, PETIM, and PETAA which are 0.798837, 0.798841, and 0.798835, respectively. For each of the four structures, a graph as shown in Figure 6 is plotted against the values found in Table 7.

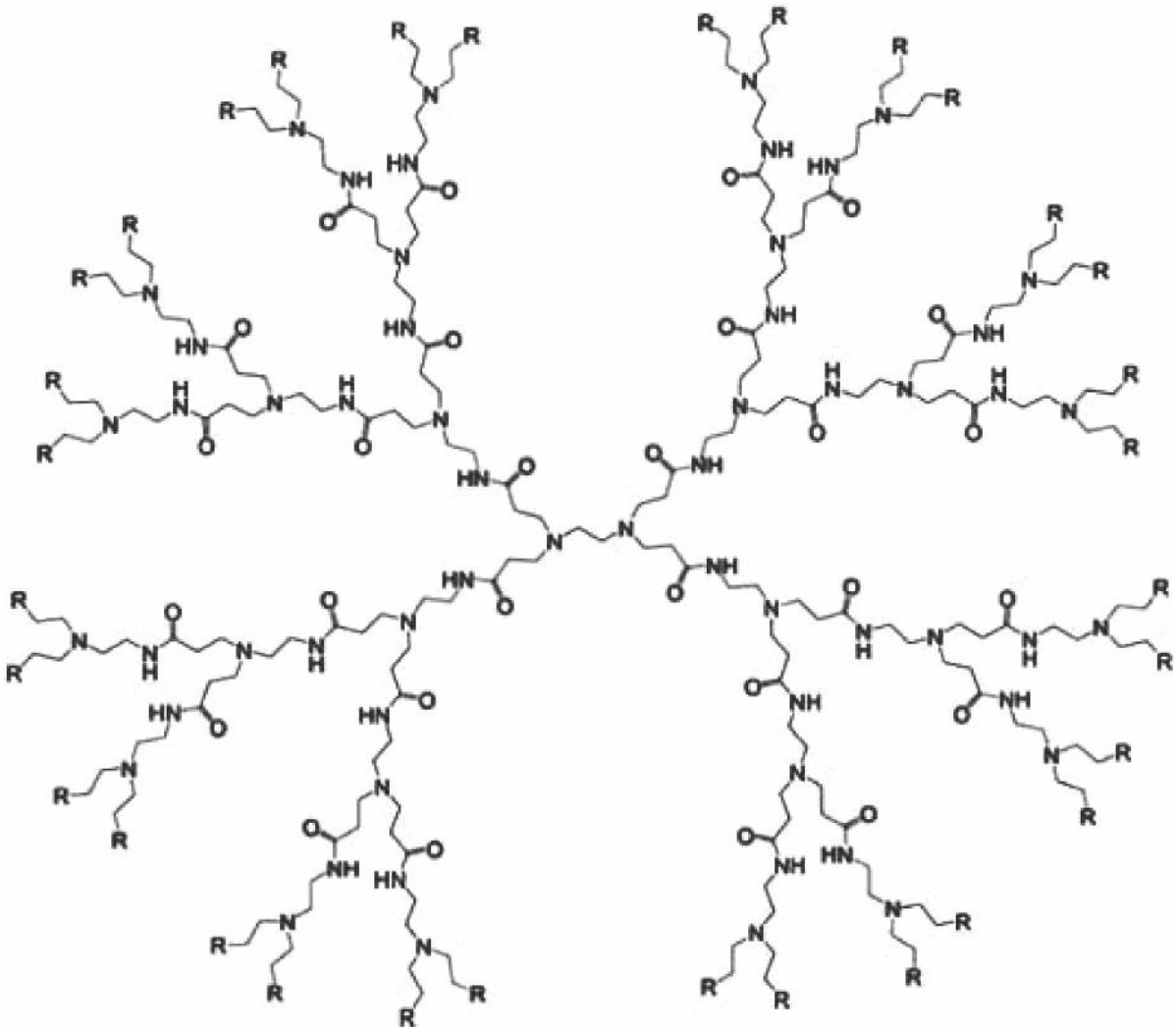


Figure 5: The molecular graph of polyethylene amide amine dendrimer.

Table 6: Edge partition of PETAA.

(d_v, d_ω), where $v\omega \in E(G)$	$(1,2)$	$(1,3)$	$(2,2)$	$(2,3)$
Number of edges	4×2^n	$4 \times 2^n - 2$	$16 \times 2^n - 8$	$20 \times 2^n - 9$

As the SS index is found to have very good correlation coefficient $r = 0.99 \cong 1$ with the above-discussed physicochemical properties, the novel index is of great use in the QSPR/QSAR/QSTR analysis by the chemists.

5. Mathematical Properties of SS Index

In this section, the SS indexes of cycle, star, path, and simple graphs are computed [34–38].

Theorem 5. *For a cycle C_n, where n is the cardinality of vertices, then the SS index of C_n is given by $SS(C_n) = n$.*

Proof. A cycle C_n has n vertices and n edges. The n edges of the cycle will be of type (2, 2). By considering all the n edges and using the definition of SS index, we get $SS(C_n) = n$. □

Theorem 6. *For a star S_n, where n is the cardinality of vertices, then the SS index of S_n is given by*

$$SS(S_n) = \frac{(n-1)^{3/2}}{\sqrt{n}}. \tag{14}$$

Proof. A star S_n has n vertices and $(n-1)$ edges. The $(n-1)$ edges of the star graph will be of type $(1, n-1)$. By considering all the $(n-1)$ edges and using the definition of SS index, we get

$$SS(S_n) = \frac{(n-1)^{3/2}}{\sqrt{n}}. \tag{15}$$

□

Table 7: Numerical comparison of SS(D_nP_n), SS(DPZ$_n$), SS(PETIM), and SS(PETAA) for $n = 1$ to 10.

n	1	2	3	4	5	6	7	8	9	10
D_nP_n	100.60	212.78	324.95	437.13	549.31	661.48	773.66	885.84	998.01	1110.2
DPZ$_n$	92.252	231.48	509.95	1066.9	2180.7	4408.4	8863.9	17775	35596	71240
PETIM	23.84	72.251	169.07	362.72	750.02	1524.6	3073.8	6172.2	12369	24762
PETTA	37.69	94.97	209.53	438.65	896.89	1813.4	3646.3	7312.2	14644	29308

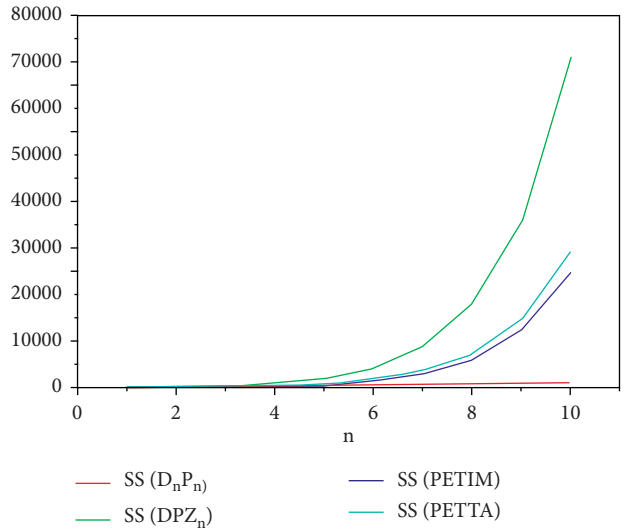


Figure 6: Graphical comparison of SS(D_nP_n), SS(DPZ$_n$), SS(PETIM), and SS(PETAA) for $n = 1$ to 10.

Theorem 7. *For a path P_n, where n is the cardinality of vertices, then the SS index of P_n is given by $SS(P_n) = (n-3) + (2\sqrt{2}/\sqrt{3})$.*

Proof. A path P_n has n vertices and $(n-1)$ edges. The $(n-1)$ edges of the path graph will be 2 edges of type (1, 2) and $(n-3)$ edges of type (2, 2), respectively. By considering all the $(n-1)$ edges and using the definition of SS index, we get $SS(P_n) = (n-3) + (2\sqrt{2}/\sqrt{3})$.

The SS indexes of cycle, star, and path graphs are related as follows:

$$SS(S) = \frac{(n-1)^{3/2}}{\sqrt{SS(C_n)}}, \qquad SS(P_n) = SS(C_n) + \frac{2\sqrt{2}}{\sqrt{3}} - 3. \tag{16}$$

□

Theorem 8. *Consider a simple graph G with m edges and cardinality n. Let p, , and δ_1 be the pendent vertices and maximum and minimum vertex degrees of G, respectively. Then,*

$$SS(G) \geq \frac{p\sqrt{\delta_1}}{\sqrt{1+\delta_1}} + \frac{2\sqrt{n\delta_1\Delta}}{\Delta+\delta_1}\sqrt{ISI(G) - \frac{p\delta_1}{1+\delta_1}}. \tag{17}$$

Proof. For $2 \leq \delta_1 \leq d_v, d_\omega \leq \Delta$,

$$\frac{d_v d_\omega}{d_v + d_\omega} \leq \frac{\Delta}{2}, \tag{18}$$

such that the equality holds iff $d_v = d_\omega = \Delta$. Also,

$$\frac{d_v d_\omega}{d_v + d_\omega} \geq \frac{\delta_1}{2}, \tag{19}$$

with equality holding if $d_v = d_\omega = \delta_1$. Using Polya–Szego inequality,

$$\left(\sum_{vw\in E(G):\, d_v, d_w \neq 1} \sqrt{\frac{d_v d_\omega}{d_v + d_\omega}}\right)^2 \geq \frac{4n\delta_1\Delta}{(\Delta+\delta_1)^2}\left(\sum_{vw\in E(G):\, d_v, d_w \neq 1} \frac{d_v d_\omega}{d_v + d_\omega}\right) \geq \frac{4n\delta_1\Delta}{(\Delta+\delta_1)^2}\left(ISI(G) - \sum_{vw\in E(G):\, d_v = 1} \frac{d_\omega}{1+d_\omega}\right),$$
$$\left(\sum_{vw\in E(G):\, d_v, d_w \neq 1} \sqrt{\frac{d_v d_\omega}{d_v + d_\omega}}\right) \geq \frac{2\sqrt{n\delta_1\Delta}}{(\Delta+\delta_1)}\sqrt{ISI(G) - \frac{p\delta_1}{1+\delta_1}}, \tag{20}$$

we have

$$SS(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_w}{1+d_w}} + \left(\sum_{vw \in E(G):\, d_v, d_w \neq 1} \sqrt{\frac{d_v d_\omega}{d_v + d_\omega}} \right). \tag{21}$$

For $\Delta \geq d_v$, from (20) and (21), we get

$$SS(G) \geq \frac{p\sqrt{\delta_1}}{\sqrt{1+\delta_1}} + \frac{2\sqrt{n\delta_1\Delta}}{\Delta+\delta_1} \sqrt{ISI(G) - \frac{p\delta_1}{1+\delta_1}}. \tag{22}$$

□

Theorem 9. *For a tree T with cardinality n and pendent vertices p, then the SS index is*

$$SS(T) \geq \frac{p\sqrt{\delta_1}}{\sqrt{1+\delta_1}} + \frac{2\sqrt{(m-1)\delta_1\Delta}}{\Delta+\delta_1} \sqrt{ISI(G) - \frac{p\delta_1}{1+\delta_1}}. \tag{23}$$

Theorem 10. *Consider simple graph G of order n with m edges and cardinality n. Here, p, , and δ_1 represent pendent vertices and maximum vertex degree and minimum non-pendent vertex degree, respectively, and then*

$$SS(G) \leq \frac{p\sqrt{\Delta}}{\sqrt{1+\Delta}} + \sqrt{(m-p)\left[ISI(G) - \frac{p\Delta}{1+\Delta} \right]}. \tag{24}$$

Proof. By Cauchy–Schwarz inequality,

$$\begin{aligned}
\left(\sum_{vw \in E(G):\, d_v, d_w \neq 1} \sqrt{\frac{d_v d_\omega}{d_v + d_\omega}} \right)^2 &\leq (m-p) \left(\sum_{vw \in E(G):\, d_v, d_w \neq 1} \frac{d_v d_\omega}{d_v + d_\omega} \right), \\
&\leq (m-p) \left[ISI(G) - \sum_{vw \in E(G):\, d_v = 1} \frac{d_\omega}{1+d_\omega} \right] \\
&\leq (m-p) \left[ISI(G) - \frac{p\Delta}{1+\Delta} \right] \\
\left(\sum_{vw \in E(G):\, d_v, d_w \neq 1} \sqrt{\frac{d_v d_\omega}{d_v + d_\omega}} \right) &\leq \sqrt{(m-p)\left(ISI(G) - \frac{p\Delta}{1+\Delta} \right)} \\
SS(G) &\leq \frac{p\sqrt{\Delta}}{\sqrt{1+\Delta}} + \sqrt{(m-p)\left[ISI(G) - \frac{p\Delta}{1+\Delta} \right]}.
\end{aligned} \tag{25}$$

□

Theorem 11. *The cardinality n of a tree T and pendent vertices p and then the SS index is*

$$SS(T) \leq \frac{p\sqrt{\Delta}}{\sqrt{1+\Delta}} + \sqrt{(n-1-p)\left[ISI(G) - \frac{p\Delta}{1+\Delta} \right]}. \tag{26}$$

6. Conclusion

In this article, a novel index known as SS index is introduced and computed for four dendrimers such as D_nP_n, DPZ_n, PETIM, and PETAA. To validate the performance of this novel index, the chemical applicability of 67 alkane isomers is studied. It is observed that the proposed index has a very good correlation with alkane isomers considered in the study. The results obtained for the dendrimers have proved that they play a major role in drugs including anti-inflammatory, antimicrobial, and anticancer in administering the drug. Dendrimers play a vital role in the discovery of drugs against the diseases such as Alzheimer's, HIV, and cancer. The article is concluded by mathematical properties of SS iindexes for cycle, star, path, and simple graphs.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

All the authors contributed equally to this study. M. C. Shanmukha gave the idea and wrote the manuscript. A. Usha and K. C. Shilpa edited and verified the results. Weidong Zhao checked and corrected the initial manuscript and verified the results. M. Reza Farahani added some final

remarks and improved the overall paper. All authors read and approved the final draft.

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