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ON AUGMENTED REVERSE INDEX AND ITS POLYNOMIAL OF CERTAIN NANOSTAR DENDRIMERS

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ABSTRACT

Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of the Chemical Sciences. In this paper, we introduce the augmented reverse index and augmented reverse polynomial of a molecular graph. Also we compute the augmented reverse index and its polynomial of certain important nanostar dendrimers.

Keywords: *augmented reverse index, augmented reverse polynomial, dendrimer.*
Mathematics Subject Classification: *05C05, 05C12, 05C35.*

I. INRTODUCTION

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The degree $\Delta(G)$ denote the largest of all degrees of G. The reverse degree of a vertex v in G is defined as $c_v = \Delta(G) - d_G(v) + 1$. The reverse edge connecting the vertices u and v will be denoted by uv.We refer to [1] for undefined term and notation.

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. Numerous topological indices are useful for establishing correlations between the structure of a molecular compound and its physico-chemical properties, see [2].

Furtula et al. proposed augmented Zagreb index, defined as [3]

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u)d_G(v)}{d_G(u) + d_G(v) - 2} \right)^3 .$$

This topological index has proved to a valuable predictive index in the study of the heat formation in octanes and heptanes, whose prediction power is better than atom bond connectivity index, see [3]. This index was also studied, for example, in [4, 5, 6, 7, 8].

We now introduce the augmented reverse index, defined as

$$ACI(G) = \sum_{uv \in E(G)} \left(\frac{c_u c_v}{c_u + c_v - 2} \right)^3 .$$

Considering the augmented reverse index, we define the augmented reverse polynomial as

$$ACI(G, x) = \sum_{uv \in E(G)} x^{\left(\frac{c_u c_v}{c_u + c_v - 2} \right)^3} .$$

Recently, many topological indices were studied, for example, in [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19].

In this paper, we compute the augmented reverse index and its polynomial of certain nanostar dendrimers. For more information about nanostar dendrimers see [20, 21, 22].

II. RESULTS FOR $NS_1[n]$ DENDRIMER NANOSTARS

In this section, we focus on the polypropylenimine octaamine dendrimer, denoted by $NS_1[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_1[n]$ nanostar dendrimer is presented in Figure 1.

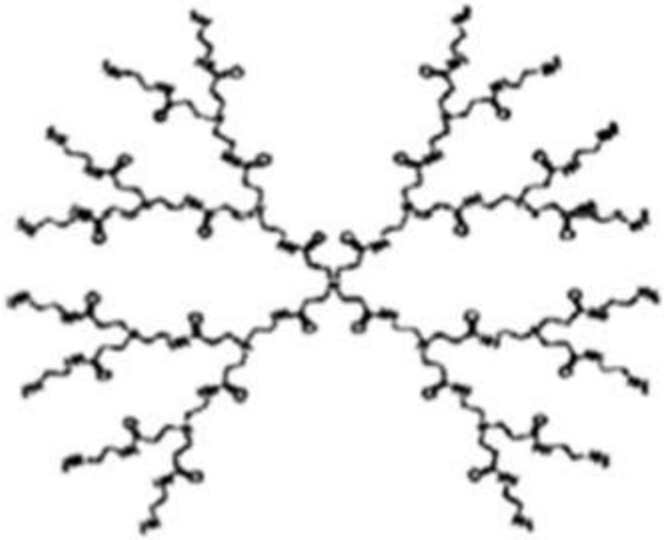

Figure 1. The molecular graph of $NS_1[n]$

Let G be the graph of polypropylenimine octaamine dendrimer $NS_1[n]$. By calculation, we obtain that G has $32 \times 2^n - 29$ edges. From Figure 1, it is easy to see that the vertices of NS_1[n] are either of degree 1, 2 or 3.

Therefore $\Delta(G) = 3$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 4 - d_G(u)$. Also by calculation, we obtain that the edge set $E(NS_1[n])$ can be divided into four partitions based on the degree of end vertices of each edge as follows:

$E_{12} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_{12}| = 2 \times 2^n$.
$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_{13}| = 4 \times 2^n - 4$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 12 \times 2^n - 11$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 14 \times 2^n - 14$.

Thus there are four types of reverse edges based on the reverse degree of end reverse vertices of each reverse edge as given in Table 1.

Table 1. Reverse edge partition of $NS_1[n]$

$c_u, c_v \backslash uv \in E(G)$	(3, 2)	(3, 1)	(2,2)	(2,1)
Number of edges	2×2^n	$4 \times 2^n - 4$	$12 \times 2^n - 11$	$14 \times 2^n - 14$

In the following theorems, we compute the augmented reverse index and augmented reverse polynomial of $NS_1[n]$.

Theorem 1. The augmented reverse index of a polypropylenimine octaamine dendrimer $NS_1[n]$ is given by

$$ACI\left(NS_1[n]\right) = \frac{1}{2}\left(475 \times 2^n - 427\right).$$

Proof: Let G be the graph of $NS_1[n]$. By using equation (1) and using Table 1, we deduce

$$ACI\left(NS_1[n]\right) = \sum_{uv \in E(G)} \left(\frac{c_u c_v}{c_u + c_v - 2}\right)^3$$

$$= \left(\frac{3\times2}{3+2-2}\right)^3 2\times2^n + \left(\frac{3\times1}{3+1-2}\right)^3 \left(4\times2^n - 4\right) + \left(\frac{2\times2}{2+2-2}\right)^3 \left(12\times2^n - 11\right)$$

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$$+\left(\frac{2\times 1}{2+1-2}\right)^3\left(14\times 2^n-14\right)$$
$$=\frac{1}{2}\left(475\times 2^n-427\right).$$

Theorem 2. The augmented reverse polynomial of a polypropylenimine octaamine dendrimer $NS_1[n]$ is given by

$$ACI\left(NS_1[n],x\right)=\left(4\times 2^n-4\right)x^{\frac{27}{8}}+\left(28\times 2^n-25\right)x^8.$$

Proof: Let G be the graph of $NS_1[n]$. By using equation (2) and using Table 1, we deduce

$$ACI\left(NS_1[n],x\right)=\sum_{uv\in E(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3}$$

$$=2\times 2^n x^{\left(\frac{3\times 2}{3+2-2}\right)^3}+\left(4\times 2^n-4\right)x^{\left(\frac{3\times 1}{3+1-2}\right)^3}+\left(12\times 2^n-11\right)x^{\left(\frac{2\times 2}{2+2-2}\right)^3}+\left(14\times 2^n-14\right)x^{\left(\frac{2\times 1}{2+1-2}\right)^3}$$
$$=2\times 2^n x^8+\left(4\times 2^n-4\right)x^{\frac{27}{8}}+\left(12\times 2^n-11\right)x^8+\left(14\times 2^n-14\right)x^8$$
$$=\left(4\times 2^n-4\right)x^{\frac{27}{8}}+\left(28\times 2^n-25\right)x^8.$$

III. RESULTS FOR DENDRIMERSNANOSTARS$NS_2[n]$

In this section, we focus on the polypropylenimine octaamine dendrimer, denoted by $NS_2[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_2[n]$ dendrimer nanostar is presented in Figure 2.

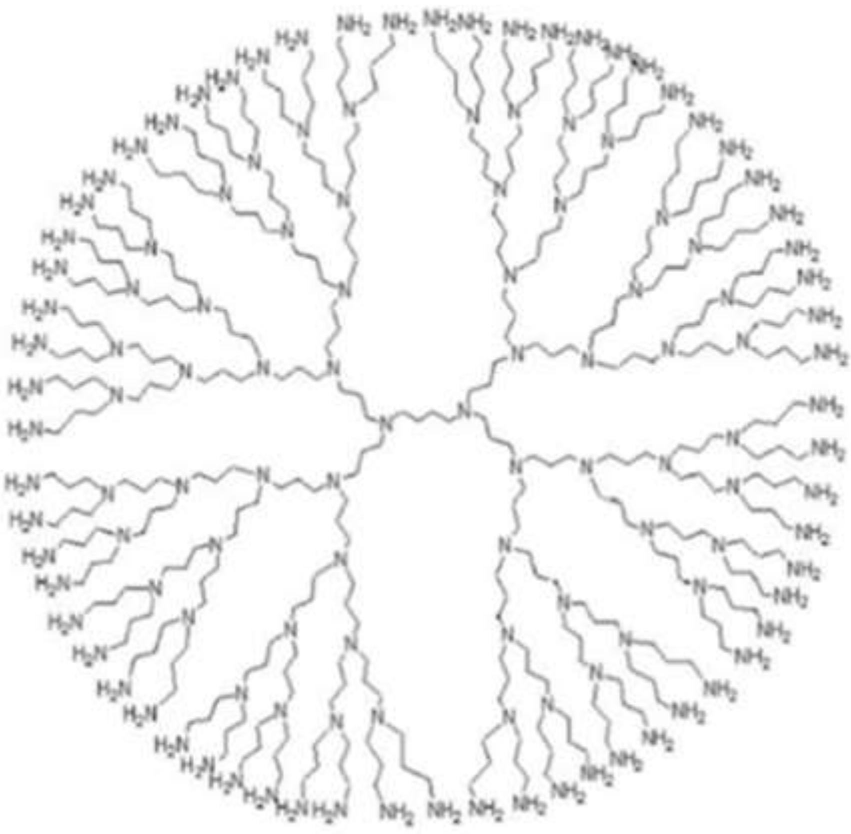

Figure 2. The structure of $NS_2[n]$

Let G be the graph of polypropylenimine octaamine dendrimer $NS_2[n]$. By calculation, we obtain that G has $16 \times 2^n - 11$ edges. From Figure 2, it is easy to see that the vertices of $NS_2[n]$ are either of degree 1, 2 or 3.

Therefore $\Delta(G) = 3$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 4 - d_G(u)$. Also by calculation, we obtain that the edge set $E(NS_2[n])$ can be divided into three partitions based on the degree of end vertices of each edge as follows:

$E_{12} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_{12}| = 2 \times 2^n$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 8 \times 2^n - 5$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 6 \times 2^n - 6$.

Thus there are three types of reverse edges based on the reverse degree of end reverse vertices of each reverse edge as given in Table 2.

Table 2. Reverse edge partition of $NS_2[n]$

$c_u, c_v \setminus uv \in \in E(G)$	(3, 2)	(2,2)	(2,1)
Number of edges	2×2^n	$8 \times 2^n - 5$	$6 \times 2^n - 6$

We now determine the augmented reverse index of $NS_2[n]$.

Theorem 3. The augmented reverse index of a polypropylenimine octaamine dendrimer $NS_2[n]$ is given by

$$ACI\left(NS_2[n]\right) = 8\left(16 \times 2^n - 11\right).$$

Proof: Let G be the graph of $NS_2[n]$. By using equation (1) and using Table 2, we deduce

$$ACI\left(NS_2[n]\right) = \sum_{uv \in E(G)} \left(\frac{c_u c_v}{c_u + c_v - 2}\right)^3$$

$$= \left(\frac{3\times2}{3+2-2}\right)^3 2\times2^n + \left(\frac{2\times2}{2+2-2}\right)^3 \left(8\times2^n - 5\right) + \left(\frac{2\times1}{2+1-2}\right)^3 \left(6\times2^n - 6\right)$$

$$= 8\left(16\times2^n - 11\right).$$

In the following theorem, we determine the augmented reverse polynomial of $NS_2[n]$.

Theorem 4. The augmented reverse polynomial of a polypropylenimine octaamine dendrimer $NS_2[n]$ is given by

$$ACI\left(NS_2[n], x\right) = \left(16\times2^n - 11\right)x^8.$$

Proof: Let G be the graph of $NS_2[n]$. By using equation (2) and using Table 2, we deduce

$$ACI\left(NS_2[n], x\right) = \sum_{uv \in E(G)} x^{\left(\frac{c_u c_v}{c_u + c_v - 2}\right)^3}$$

$$= 2\times2^n x^{\left(\frac{3\times2}{3+2-2}\right)^3} \left(8\times2^n - 5\right) x^{\left(\frac{2\times2}{2+2-2}\right)^3} + \left(6\times2^n - 6\right) x^{\left(\frac{2\times1}{2+1-2}\right)^3}$$

$$= \left(16\times2^n - 11\right)x^8.$$

IV. RESULTS FOR $NS_3[n]$ DENDRIMER NANOSTARS

In this section, we focus on the molecular graph structure of the first class of dendrimer nanostars. This family of dendrimer nanostars is denoted by $NS_3[n]$, where n is the steps of growth in this type of dendrimer nanostars. The molecular graph structure of $NS_3[3]$ dendrimer nanostar is presented in Figure 3.

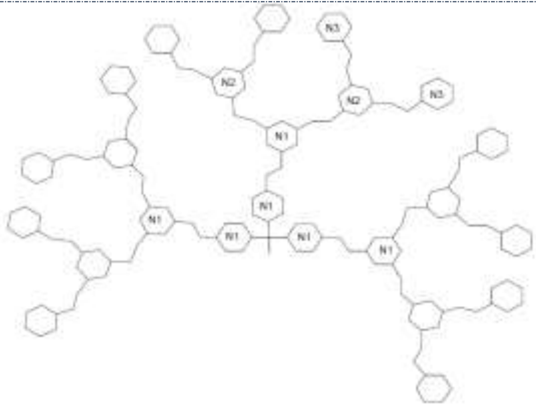

Figure 3. The structure of $NS_3[3]$

Let G be the molecular graph of a dendrimer nanostar $NS_3[n]$. By calculation, we obtain that G has $27 \times 2^n - 5$ edges. From Figure 3, it is easy to see that the vertices of $NS_3[n]$ are either of degree 1, 2, 3 or 4. Therefore $\Delta(G) = 4$ and $\delta(G) = 1$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 5 - d_G(u)$. Also by calculation, we obtain that the edge set $E(NS_3[n])$ can be divided into three partitions based on the degree of end vertices of each edge as follows:

$E_{14} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 4\}$, $|E_{14}| = 1$

$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 9 \times 2^n + 3$.

$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 18 \times 2^n - 12$.

$E_{34} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_{34}| = 3$.

Thus there are four types of reverse edges based on the reverse degree of end reverse vertices of each reverse edge as given in Table 3.

Table 3. Reverse edge partition of $NS_3[n]$

$c_u, c_v \setminus uv \in E(G)$	(4, 1)	(3, 3)	(3,2)	(2,1)
Number of edges	1	$9 \times 2^n + 3$	$18 \times 2^n - 12$	3

We compute the augmented reverse index of $NS_3[n]$.

Theorem 5. The augmented reverse index of a dendrimer nanostar $NS_3[n]$ is given by

$$ACI(NS_3[n]) = \frac{13857}{64} \times 2^n - \frac{61271}{1728}.$$

Proof: Let G be the graph of $NS_3[n]$. By using equation (1) and using Table 3, we compute

$$ACI(NS_3[n]) = \sum_{uv \in E(G)} \left(\frac{c_u c_v}{c_u + c_v - 2} \right)^3$$

$$= \left(\frac{4 \times 1}{4+1-2} \right)^3 + \left(\frac{3 \times 3}{3+3-2} \right)^3 (9 \times 2^n + 3) + \left(\frac{3 \times 2}{3+2-2} \right)^3 (18 \times 2^n - 12) + \left(\frac{2 \times 1}{2+1-2} \right)^3 \times 3$$

$$= \frac{13857}{64} \times 2^n - \frac{61271}{1728}.$$

In the next theorem, we compute the augmented reverse polynomial of $NS_3[n]$.

Theorem 6. The augmented reverse polynomial of a dendrimer nanostar $NS_3[n]$ is given by

$$ACI(NS_3[n], x) = x^{\frac{64}{27}} + (9 \times 2^n + 3) x^{\frac{729}{64}} + (18 \times 2^n - 9) x^8.$$

Proof: Let G be the graph of $NS_3[n]$. By using equation (2) and using Table 3, we compute

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$$ACI\left(NS_3[n],x\right)=\sum_{uv\in E(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3}$$

$$=x^{\left(\frac{4\times1}{4+1-2}\right)^3}+\left(9\times2^n+3\right)x^{\left(\frac{3\times3}{3+3-2}\right)^3}+\left(18\times2^n-12\right)x^{\left(\frac{3\times2}{3+2-2}\right)^3}+3\times x^{\left(\frac{2\times1}{2+1-2}\right)^3}$$

$$=x^{\frac{64}{27}}+\left(9\times2^n+3\right)x^{\frac{729}{64}}+\left(18\times2^n-9\right)x^8.$$

V. RESULTS FOR DENDRIMER NANOSTARS $D_1[n]$

In this section, we consider a family of dendrimer nanostars with n growth stages, denoted by $D_1[n]$. The graph of $D_1[n]$ with 4 growth stages is depicted in Figure 4.

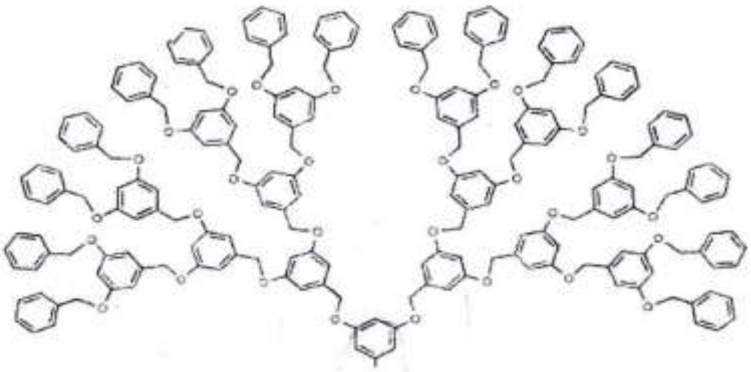

Figure 4. The molecular graph of $D_1[4]$

Let G be the graph of a dendrimer nanostar $D_1[n]$. By calculation, we obtain that G has $18 \times 2^n - 11$ edges. From Figure 4, it is easy to see that the vertices of $D_1[n]$ are either of degree 1, 2 or 3. Therefore $\Delta(G) = 3$ and $\Delta(G) = 1$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 4 - d_G(u)$. Also by calculation, we obtain that the edge set $E(D_1[n])$ can be divided into three partitions based on the degree of end vertices of each edge as follows:

$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_{13}| = 1$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 6 \times 2^n - 2$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 12 \times 2^n - 10$.

Thus there are three types of reverse edges based on the reverse degree of end reverse vertices of each reverse edge as given in Table 4.

Table 4. Reverse edge degree partition of $D_1[n]$

$c_u, c_v \setminus uv\in E(G)$	(3,1)	(2, 2)	(2, 1)
Number of edges	1	$6 \times 2^n - 2$	$12 \times 2^n - 10$

We compute the augmented reverse index of dendrimer nanostar $D_1[n]$.

Theorem 7. The augmented reverse index of a dendrimer nanostar $D_1[n]$ is given by

$$ACI\left(D_1[n]\right)=144\times2^n-\frac{741}{8}.$$

Proof: Let G be the graph of a dendrimer nanostar $D_1[n]$. By using equation (1) and using Table 4, we obtain

$$ACI\left(D_1[n]\right)=\sum_{uv\in E(G)}\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3$$

$$=\left(\frac{3\times1}{3+1-2}\right)^3+\left(\frac{2\times2}{2+2-2}\right)^3\left(6\times2^n-2\right)+\left(\frac{2\times1}{2+1-2}\right)^3\left(12\times2^n-10\right)$$

$$= 144 \times 2^n - \frac{741}{8}.$$

In the next theorem, we compute the augmented reverse polynomial of dendrimer nanostar $D_1[n]$.

Theorem 8. The augmented reverse polynomial of a dendrimer nanostar $D_1[n]$ is given by

$$ACI\left(D_1[n], x\right) = x^{\frac{27}{8}} + \left(18 \times 2^n - 12\right)x^8.$$

Proof: Let G be the graph of a dendrimer nanostar $D_1[n]$. By using equation (2) and using Table 4, we obtain

$$ACI\left(D_1[n], x\right) = \sum_{uv \in E(G)} x^{\left(\frac{c_u c_v}{c_u + c_v - 2}\right)^3}$$

$$= x^{\left(\frac{3\times 1}{3+1-2}\right)^3} + \left(6 \times 2^n - 2\right)x^{\left(\frac{2\times 2}{2+2-2}\right)^3} + \left(12 \times 2^n - 10\right)x^{\left(\frac{2\times 1}{2+1-2}\right)^3}$$

$$= x^{\frac{27}{8}} + \left(18 \times 2^n - 12\right)x^8.$$

REFERENCES

[1] V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
[2] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17, (1972) 535-538.
[3] B. Furtula, A Graovac and D. Vukičević, Augmented Zagreb index, *J. Math. Chem.* 48(2010) 370-380.
[4] V.R.Kulli, Some topological indices of certain nanotubes, *Journal of Computer and Mathematical Sciences*, 8(1), (2017) 1-7.
[5] V.R. Kulli, Computation of some topological indices of certain networks, *International Journal of Mathematical Archive,* 8(2) (2017) 99-106.
[6] V.R. Kulli, New augmented Zagreb indices, *International Journal of Mathematical Achieve*, 8(8) (2017) 102-108.
[7] V.R.Kulli, On augmented Revan index and its polynomial of certain families of benzenoid system, submitted.
[8] V.R.Kulli, On augmented ve-degree index and its polynomial of dominating oxide and regular triangulate oxide networks, submitted.
[9] V.R.Kulli, Hyper-Revan indices and their polynomials of silicates networks, *International Journal of Current Research in Science and Technology*, 4(3) (2018).
[10] V.R.Kulli, Revan indices and their polynomials of certain rhombus networks, *International Journal of Current Research in Life Sciences*, 7(5) (2018) 2110-2116.
[11] V.R. Kulli, Reverse Zagreb and reverse hyper-Zagreb indices and their polynomials of rhombus silicate networks, *Annals of Pure and Applied Mathematics,* 16(1) (2018) 47-51.
[12] V.R. Kulli, General Zagreb polynomials and F-polynomial of certain nanostructures, *International Journal of Mathematical Archive*, 8(10) (2017) 103-109.
[13] V.R.Kulli, Certain topological indices and their polynomials of dendrimer nanostars, *Annals of Pure and Applied Mathematics* 14(2) (2017) 263-268.
[14] V.R.Kulli, General fifth *M*-Zagreb indices and fifth *M*-Zagreb polynomials of PAMAM dendrimers, *International Journal of Fuzzy Mathematical Archive*, 13(1) (2017) 99-103.
[15] V.R.Kulli, F-reverse index and F-Reverse polynomial of certain families of benzenoid systems, submitted.
[16] V.R.Kulli, Computing F-Revan index and F-Revan polynomial of certain networks, submitted.
[17] V.R.Kulli, Computing F-reverse index and F-reverse polynomial of certain networks, submitted.
[18] V.R.Kulli, F-reverse index and F-reverse polynomial of certain families of benzenoid systems, submitted.
[19] V.R.Kulli, Computing the F-ve-degree index and its polynomial of dominating oxide and regular triangulate oxide networks, *International Journal of Fuzzy Mathematical Archive*, 16(1) (2018) 1-6.
[20] V.R.Kulli, Multiplicative atom bond connectivity and multiplicative geometric-arithmetic indices of chemical structures in drugs, *International Journal of Mathematical Archive*, 9(6) (2018) 155-163.
[21] N. De and S.M.A. Nayeem, Computing the *F*-index of nanostar dendrimers, *Pacific Science Review A: Natural Science and Engineering* (2016) DoI:http:/dx.doi.org/10.1016/j.psra.2016.06.001.

ISSN: 2277-9655
Impact Factor: 5.164
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[22] A.R. Ashrafi and P. Nikzad, Connectivity index of the family of dendrimer nanostars, *Digest Journal of Nanomaterials and Biostructures*, 4(2) (2009) 269-273..

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