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Degree Based Topological Indices of Zig Zag Chain

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Abstract. In this paper, we obtained the degree based topological indices like Randic, Geometric – Arithmetic, Sum Connectivity, Harmonic, First Zagreb, Second Zagreb, Second Modified Zagreb, Inverse Sum, Albertson, Atom – bond Connectivity, Symmetric – Division index and Augmented Zagreb indices for Zig-Zag chain of 8-cycles molecular graph. The degree based topological indices for the Zig- Zag chain of 8-cycles are computed as expressions in 'a' and 'n', where 'a' represents the number of hexagons and 'n' represents the number of segments.

Keywords: Topological index, molecular graph, M-polynomial, zig-zag chain of 8-cycles.

AMS Mathematics Subject Classification (2010): 05C05, 05C12

1. Introduction

In medicine mathematical model, the structure of drug is represented as an undirected graph, where each vertex indicates an atom and each edge represents a chemical bond between these atoms.

With rapid development of medicine manufacture, a large number of new drugs have been developed each year. Hence, it demands a tremendous amount of work to determine the pharmacological, chemical and biological characteristics of these new drugs, and such workloads become more and more fussy and clustered.

It requires enough reagents equipment and assistants to test the performances and the side effects of existing new drugs. However, in lower income countries and areas (such as certain cities and countries in South America, Africa and Southeast Asia), there is no sufficient money to defray reagents and equipment which can be employed to measure the biochemical properties.

Fortunately, many previous studies[1-4] have pointed that chemical and pharma codynamics characteristics of drugs and their molecular structures are closely linked. If we calculate indicators of these drug molecular structures[5-9] in view of defining the topological indices, the medical and pharmaceutical scholars could find it useful to well know their medicinal properties, which can make up the defects of medicine and chemical experiments. From this standpoint, the methods on topological index computation are very suitable and serviceable for developing countries in which they can yield the available biological and medical information of new drugs without chemical experiment hardware.

Although there have been several contributions on distance-based indices and degree-based molecular structures,[10-13] the researches of topological index for certain special drug structures are still largely limited. Because of these, tremendous academic and industrial interest has been attracted to research the topological index of drug molecular structure from a mathematical point of view.

2. Computational procedure of M-polynomial

M-Polynomial of graph G is defined as if $G=(V,E)$ is a graph and $v \in V$, then $d_v(G)$ (or d_v for short if G is clear from the context) denotes the degree of v. Let G be a graph and let $m_{ij}(G), i, j \geq 1$, be the number of edges e = uv of G such that $\{d_u(G), d_v(G)\} = \{i, j\}$ The M-polynomial of G as $M(G;x,y)=\sum_{i\leq j} m_{ij}(G)x^i y^j$ .For a graph $G=(V,E)$, a degree-based topological index is a graph invariant of the form $I(G) = \sum_{e=uv\in E} f(d_u, d_v)$ where $f = f(x,y)$ is a function appropriately selected for possible chemical applications.

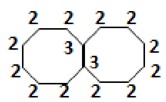
3. Some special cases

3.1. Case 1

Let 'n' be the number of rows in the Zig- Zag chain of 8- cycles $Z_8(n)$, for n=1

$\Rightarrow$ Number of hexagon = a = 2

For $Z_8(1)$, the number of edges with end degrees (2,2) is 10, the number of edges with end degrees (2,3) is 4, the number of edges with end degrees (3,3) is 1, total number of edges for n=1 is 15.

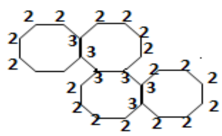


3.2. Case 2

Let 'n' be the number of rows in the Zig- Zag chain of 8- cycles $Z_8(n)$, for n=2

$\Rightarrow$ Number of hexagon = a = 4

For $Z_8(2)$, the number of edges with end degrees (2,2) is 16, the number of edges with end degrees (2,3) is 8, the number of edges with end degrees (3,3) is 5, total number of edges for n=2 is 29.

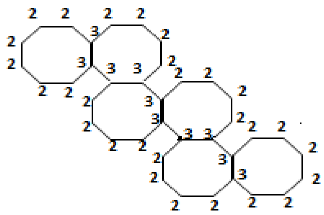


3.3. Case 3

Let 'n' be the number of rows in the Zig- Zag chain of 8- cycles $Z_8(n)$, for n=3

$\Rightarrow$ Number of hexagon = a = 6

For $Z_8(3)$, the number of edges with end degrees (2,2) is 22, the number of edges with end degrees (2,3) is 12, the number of edges with end degrees (3,3) is 9, total number of edges for n=3 is 43.

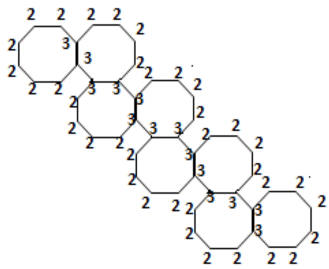


3.4. Case 4

Let ‘n’ be the number of rows in the Zig- Zag chain of 8- cycles $Z_8(n)$, for n=4

$\Longrightarrow$ Number of hexagon = a = 8

For $Z_8(4)$, the number of edges with end degrees (2,2) is 28, the number of edges with end degrees (2,3) is 16, the number of edges with end degrees (3,3) is 13, total number of edges for n=4 is 57.

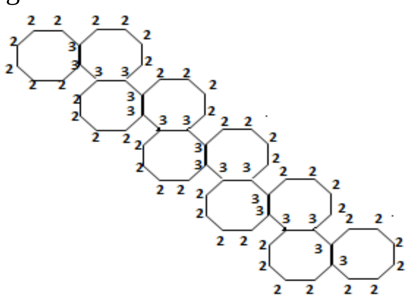


3.5. Case 5

Let ‘n’ be the number of rows in the Zig- Zag chain of 8- cycles $Z_8(n)$, for n=5

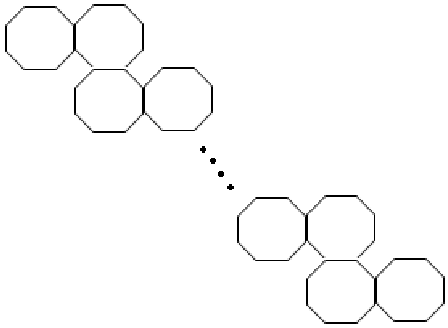
$\Longrightarrow$ Number of hexagon = a = 10

For $Z_8(n)$, the number of edges with end degrees (2,2) is 34, the number of edges with end degrees (2,3) is 20, the number of edges with end degrees (3,3) is 17, total number of edges for n=5 is 71.



4. Generalization of zig zag chain of molecular graph

For $Z_8(n)$, for $n \geq 1$, a= 2n then the number of edges with end degrees (2,2) is 6n+4, the number of edges with end degrees (2,3) is 4n, the number of edges with end degrees (3,3) is 4n-3, total number of edges for any n is given by 14n+1.



5. M-Polynomial of ZigZag chain of 8-cycles of graph

Let

$$Z_8(n) = (6n+4)x^2y^2 + (4n)x^2y^3 + (4n-3)x^3y^3 \; for \; all \; n \geq 1$$

Topological Index	$\{\varphi_{ij}\}$	**Notation**	**Topological Index**	$\{\varphi_{ij}\}$	**Notation**
Randic	$\frac{1}{\sqrt{ij}}$	$\chi(G)$	Second modified Zagreb	$\frac{1}{ij}$	$M_3(G)$
Geometric-Arithmetic	$\frac{2\sqrt{ij}}{i+j}$	$GA(G)$	Inverse sum	$\frac{ij}{i+j}$	$IS(G)$
Sum-Connectivity	$\frac{1}{\sqrt{i+j}}$	$SCI(G)$	Albertson	$\lvert i-j \rvert$	$Alb(G)$
Harmonic	$\frac{2}{i+j}$	$HI(G)$	Atom-Bond connectivity	$\sqrt{\frac{i+j-2}{ij}}$	$ABCG)$
First Zagreb	$i+j$	$M_1(G)$	Symmetric Division Index	$\frac{i^2+j^2}{ij}$	$SD(G)$
Second Zagreb	ij	$M_2(G)$	Augmented Zagreb	$\left(\frac{ij}{i+j-2}\right)^3$	$AZI(G)$

Table 1: Some Important Formulae of degree based Topological indices

Theorem 1. Let 'n' be the number of rows in the Zig-Zag chain of 8-cycles of graph Z_8(n), then Randicindex is given by $\chi(Z_8(n)) = \frac{13n + 2\sqrt{6}n + 3}{3}$

Proof: Randic Index is denoted by

$$\chi(Z_8(n)) \frac{1}{\sqrt{ij}}$$

$$=\frac{1}{\sqrt{ij}}\{6n+4\}+\frac{1}{\sqrt{ij}}\{4n\}+\frac{1}{\sqrt{ij}}\{4n-3\}$$

$$=\frac{1}{\sqrt{2*2}}\{6n+4\}+\frac{1}{\sqrt{2*3}}\{4n\}+\frac{1}{\sqrt{3*3}}\{4n-3\}$$

$$=\frac{1}{\sqrt{4}}\{6n+4\}+\frac{1}{\sqrt{6}}\{4n\}+\frac{1}{\sqrt{3*3}}\{4n-3\}=\frac{1}{\sqrt{4}}\{6n+4\}+\frac{1}{\sqrt{6}}\{4n\}+\frac{1}{\sqrt{9}}\{4n-3\}$$

$$=\frac{6n+4}{2}+\frac{4n}{\sqrt{6}}+\frac{4n-3}{3}=\frac{3(6n+4)+2(4n-3)}{6}+\frac{4n}{\sqrt{6}}=\frac{18n+12+8n-6}{6}+\frac{4n}{\sqrt{6}}$$

$$=\frac{26n+6}{6}+\frac{4n}{\sqrt{6}}=\frac{26n+6}{\sqrt{6}\sqrt{6}}+\frac{4n}{\sqrt{6}}=\frac{26n+6+4n(\sqrt{6})}{6}=\frac{13n+2\sqrt{6}n+3}{3}$$

$$\chi(Z_8(n))=\frac{13n+2\sqrt{6}n+3}{3}$$

Theorem 2. Let ‘n’ be the number of rows in the Zig-Zag chain of 8-cycles of graph $Z_8(n)$, then Geometric-Arithmetic index is given by $GA(Z_8(n))=\frac{1}{5}(50n+5+8n\sqrt{6})$

Proof: Geometric – Arithmetic Index is denoted by

$$GA(Z_8(n))=\frac{2\sqrt{ij}}{i+j}$$

$$=\frac{2\sqrt{ij}}{i+j}\{6n+4\}+\frac{2\sqrt{ij}}{i+j}\{4n\}+\frac{2\sqrt{ij}}{i+j}\{4n-3\}$$

$$=\frac{2\sqrt{2*2}}{2+2}(6n+4)+\frac{2\sqrt{2*3}}{2+3}\{4n\}+\frac{2\sqrt{3*3}}{3+3}\{4n-3\}$$

$$=\frac{2\sqrt{4}}{4}(6n+4)+\frac{2\sqrt{6}}{5}\{4n\}+\frac{2\sqrt{9}}{6}\{4n-3\}=(6n+4)+\frac{2\sqrt{6}}{5}\{4n\}+\{4n-3\}$$

$$=(6n+4)+\frac{8n\sqrt{6}}{5}+\{4n-3\}=10n+1+\frac{8n\sqrt{6}}{5}$$

$$GA(Z_8(n))=\frac{1}{5}(50n+5+8n\sqrt{6})$$

Theorem 3. Let ‘n’ be the number of rows in the Zig-Zag chain of 8-cycles of graph $Z_8(n)$, then Sum-Connectivity index is given by

$$SCI(Z_8(n))=\frac{3\sqrt{30}n+2\sqrt{30}-3\sqrt{5}+4\sqrt{6}n+4\sqrt{5}n}{\sqrt{30}}$$

Proof:

Sum – Connectivity is denoted by $SCI(Z_8(n)) = \dfrac{1}{\sqrt{i+j}}$

$$=\frac{1}{\sqrt{i+j}}\{6n+4\}+\frac{1}{\sqrt{i+j}}\{4n\}+\frac{1}{\sqrt{i+j}}\{4n-3\}$$

$$=\frac{1}{\sqrt{2+2}}\{6n+4\}+\frac{1}{\sqrt{2+3}}\{4n\}+\frac{1}{\sqrt{3+3}}\{4n-3\}$$

$$=\frac{1}{\sqrt{4}}\{6n+4\}+\frac{1}{\sqrt{5}}\{4n\}+\frac{1}{\sqrt{3+3}}\{4n-3\}=\frac{1}{2}\{6n+4\}+\frac{1}{\sqrt{5}}\{4n\}+\frac{1}{\sqrt{6}}\{4n-3\}$$

$$=\frac{6n}{2}+\frac{4}{2}+\frac{4n}{\sqrt{5}}+\frac{4n}{\sqrt{6}}-\frac{3}{\sqrt{6}}=3n+2-\frac{3}{\sqrt{6}}+\frac{4n}{\sqrt{5}}+\frac{4n}{\sqrt{6}}=3n+2-\frac{3}{\sqrt{6}}+\frac{4n}{\sqrt{5}}+\frac{4n}{\sqrt{6}}$$

$$SCI(Z_8(n))=\frac{3\sqrt{30}n+2\sqrt{30}-3\sqrt{5}+4\sqrt{6}n+4\sqrt{5}n}{\sqrt{30}}$$

Theorem 4. Let 'n' be the number of rows in the Zig-Zag chain of 8-cycles of graph $Z_8(n)$, then Harmonic index is given by $HI(Z_8(n)) = \dfrac{89n+15}{15}$

Proof:

Harmonic index is denoted by $HI(Z_8(n)) = \dfrac{2}{i+j}$

$$=\frac{2}{i+j}\{6n+4\}+\frac{2}{i+j}\{4n\}+\frac{2}{i+j}\{4n-3\}$$

$$=\frac{2}{2+2}\{6n+4\}+\frac{2}{2+3}\{4n\}+\frac{2}{3+3}\{4n-3\}$$

$$=\frac{2}{4}\{6n+4\}+\frac{2}{5}\{4n\}+\frac{2}{3+3}\{4n-3\}=\frac{1}{2}\{6n+4\}+\frac{2}{5}\{4n\}+\frac{2}{3+3}\{4n-3\}$$

$$=\frac{6n}{2}+\frac{4}{2}+\frac{8n}{5}+\frac{8n}{6}-\frac{6}{6}=3n+2+\frac{8n}{5}+\frac{4n}{3}-1=3n+1+\frac{8n}{5}+\frac{4n}{3}$$

$$=\frac{45n+15+20n+24n}{15}$$

$$HI(Z_8(n))=\frac{89n+15}{15}$$

Theorem 5. Let 'n' be the number of rows in the Zig-Zag chain of 8-cycles of graph $Z_8(n)$, then first Zagreb index is given by $M_1(Z_8(n)) = 68n-2$

Proof: First Zagreb Index is denoted by $M_1(Z_8(n)) = i + j$

$= (i+j)\{6n+4\} + (i+j)\{4n\} + (i+j)\{4n-3\}$

$= (2+2)\{6n+4\} + (2+3)\{4n\} + (3+3)\{4n-3\}$

$= (4)\{6n+4\} + (5)\{4n\} + (3+3)\{4n-3\} = (4)\{6n+4\} + \{20n\} + (6)\{4n-3\}$

$= 24n + 16 + 20n + 24n - 18$

$M_1(Z_8(n)) = 68n - 2$

Theorem 6. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Second Zagreb index is given by $M_2(Z_8(n)) = 84n - 11$

Proof: Second Zagreb index is denoted by $M_2(Z_8(n)) = ij$

$= (ij)\{6n+4\} + (ij)\{4n\} + (ij)\{4n-3\} = (2*2)\{6n+4\} + (2*3)\{4n\} + (3*3)\{4n-3\}$

$= (4)\{6n+4\} + (6)\{4n\} + (3*3)\{4n-3\} = 24n + 16 + 24n + 36n - 27$

$M_2(Z_8(n)) = 84n - 11$

Theorem 7. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Second Modified Zagreb index is given by $M_3(Z_8(n)) = \frac{141n}{54} - \frac{4}{3}$

Proof: Second Modified Zagreb index is denoted by $M_3(Z_8(n)) = \frac{1}{ij}$

$$= \frac{1}{ij}\{6n+4\} + \frac{1}{ij}\{4n\} + \frac{1}{ij}\{4n-3\} = \frac{1}{2*2}\{6n+4\} + \frac{1}{2*3}\{4n\} + \frac{1}{3*3}\{4n-3\}$$

$$= \frac{1}{4}\{6n+4\} + \frac{1}{6}\{4n\} + \frac{1}{3*3}\{4n-3\} = \frac{6n+4}{4} + \frac{4n}{6} + \frac{4n-3}{9} = \frac{3n}{2} + 1 + \frac{2n}{3} + \frac{4n}{9} - \frac{3}{9}$$

$$= \frac{3n}{2} + \frac{2n}{3} + \frac{4n}{9} - \frac{1}{3} + 1 = \frac{3n}{2} + \frac{2n}{3} + \frac{4n}{9} - \frac{4}{3} = \frac{9n+4n}{6} + \frac{4n}{9} - \frac{4}{3} = \frac{13n}{6} + \frac{4n}{9} - \frac{4}{3}$$

$$= \frac{117n + 24n}{54} - \frac{4}{3}$$

$$M_3(Z_8(n)) = \frac{141n}{54} - \frac{4}{3}$$

Theorem 8. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Inverse sum index is given by $IS(Z_8(n)) = \frac{168n - 5}{10}$

Proof: Inverse Sum Index is denoted by

$$IS(Z_8(n)) = \frac{ij}{i+j}$$

$$=\frac{ij}{i+j}\{(6n+4\}+\frac{ij}{i+j}\{4n\}+\frac{ij}{i+j}\{4n-3\}$$

$$=\frac{2*2}{2+2}\{6n+4\}+\frac{2*3}{2+3}\{4n\}+\frac{3*3}{3+3}\{4n-3\}$$

$$=\frac{4}{4}\{6n+4\}+\frac{6}{5}\{4n\}+\frac{9}{6}\{4n-3\}=6n+4+\frac{24n}{5}+\frac{36n}{6}-\frac{27}{6}$$

$$=6n+4+\frac{24n}{5}+6n-\frac{9}{2}=6n+6n+\frac{24n}{5}+4-\frac{9}{2}=12n+\frac{24n}{5}+4-\frac{9}{2}=\frac{84n}{5}-\frac{1}{2}$$

$$IS(Z_8(n))=\frac{168n-5}{10}$$

Theorem 9. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Albertson index is given by $Alb(Z_8(n))=4n$

Proof: Albertson index $Alb(Z_8(n))=|i-j|$

$$=|i-j|\{6n+4\}+|i-j|\{4n\}+|i-j|\{4n-3\}$$

$$=|2-2|\{6n+4\}+|2-3|\{4n\}+|3-3|\{4n-3\},\ Alb(Z_8(n))=4n$$

Theorem 10. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Atom-Bond connectivity index is given by

$$ABC\ (Z_8(n))=\frac{15\sqrt{2}n+6\sqrt{2}+8n-6}{3}$$

Proof: Atom Bomb Connectivity

$$ABC(Z_8(n))=\sqrt{\frac{i+j-2}{ij}}$$

$$=\sqrt{\frac{i+j-2}{ij}}\{6n+4\}+\sqrt{\frac{i+j-2}{ij}}\{4n\}+\sqrt{\frac{i+j-2}{ij}}\{4n-3\}$$

$$=\sqrt{\frac{2+2-2}{2*2}}\{6n+4\}+\sqrt{\frac{2+3-2}{2*3}}\{4n\}+\sqrt{\frac{3+3-2}{3*3}}\{4n-3\}$$

$$=\sqrt{\frac{2}{4}}\{6n+4\}+\sqrt{\frac{3}{6}}\{4n\}+\sqrt{\frac{4}{9}}\{4n-3\}=\sqrt{\frac{1}{2}}\{6n+4\}+\sqrt{\frac{1}{2}}\{4n\}+\frac{2}{3}\{4n-3\}$$

$$=\sqrt{\frac{1}{2}}\{6n+4\}+\sqrt{\frac{1}{2}}\{4n\}+\frac{2}{3}\{4n-3\}=\frac{1}{\sqrt{2}}\{6n+4\}+\frac{1}{\sqrt{2}}\{4n\}+\frac{2}{3}\{4n-3\}$$

$$=\frac{6n+4}{\sqrt{2}}+\frac{4n}{\sqrt{2}}+\frac{2(4n-3)}{3}=\frac{10n+4}{\sqrt{2}}+\frac{8n-6}{3}=\frac{2(5n+2)}{\sqrt{2}}+\frac{8n-6}{3}$$

$$=\frac{\sqrt{2}\sqrt{2}(5n+2)}{\sqrt{2}}+\frac{8n-6}{3}=\sqrt{2}(5n+2)+\frac{8n-6}{3}$$

$$ABC(Z_8(n)) = \frac{15\sqrt{2}n + 6\sqrt{2} + 8n - 6}{3}$$

Theorem 11. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Symmetric Division Index is given by $SD(Z_8(n)) = \frac{86n+6}{3}$

Proof: Symmetric Division Index is denoted by

$$SD(Z_8(n)) = \frac{i^2 + j^2}{ij}$$

$$= \frac{i^2 + j^2}{ij}\{6n+4\} + \frac{i^2 + j^2}{ij}\{4n\} + \frac{i^2 + j^2}{ij}\{4n-3\}$$

$$= \frac{(2)^2 + (2)^2}{2*2}\{6n+4\} + \frac{(2)^2 + (3)^2}{2*3}\{4n\} + \frac{(3)^2 + (3)^2}{3*3}\{4n-3\}$$

$$= \frac{4+4}{4}\{6n+4\} + \frac{4+9}{6}\{4n\} + \frac{9+9}{9}\{4n-3\} = \frac{8}{4}\{6n+4\} + \frac{52n}{6} + \frac{18}{9}\{4n-3\}$$

$$= 12n + 8 + 8n - 6 + \frac{52n}{6} = 20n + 2 + \frac{52n}{6} = \frac{120n + 12 + 52n}{6} = \frac{60n + 2 + 26n}{3}$$

$$SD(Z_8(n)) = \frac{86n+6}{3}$$

Theorem 12. Let 'n' be the number of rows in the Zig -Zag chain of 8-cycles of graph $Z_8(n)$, then Augmented Zagreb index is given by $AZI(Z_8(n)) = \frac{8036n - 139}{64}$

Proof: Augmented Zagreb index is denoted by

$$AZI(Z_8(n)) = \left(\frac{ij}{i+j-2}\right)^3$$

$$= \left(\frac{ij}{i+j-2}\right)^3\{6n+4\} + \left(\frac{ij}{i+j-2}\right)^3\{4n\} + \left(\frac{ij}{i+j-2}\right)^3\{4n-3\}$$

$$= \left(\frac{2*2}{2+2-2}\right)^3\{6n+4\} + \left(\frac{2*3}{2+3-2}\right)^3\{4n\} + \left(\frac{3*3}{3+3-2}\right)^3\{4n-3\}$$

$$= \left(\frac{4}{2}\right)^3\{6n+4\} + \left(\frac{6}{3}\right)^3\{4n\} + \left(\frac{3*3}{4}\right)^3\{4n-3\}$$

$$= (2)^3\{6n+4\} + (2)^3\{4n\} + \left(\frac{9}{4}\right)^3\{4n-3\}$$

$$= (8)\{6n+4\} + (8)\{4n\} + \left(\frac{9}{4}\right)^3\{4n-3\} = 48n + 32 + 32n + \left(\frac{729}{64}\right)^3\{4n-3\}$$

$$=80n+32+\left(\frac{729}{64}\right)^3\{4n-3\}=\frac{5120n+2048-2916n-2187}{64}$$

$$AZI(Z_8(n))=\frac{8036n-139}{64}$$

6. Conclusion

Due to the quarrelsome evolving infections or viruses, a great deal of new diseases can be exposed every year. This necessitates us to develop more new drugs to indulgence new diseases. Topological indices were bring together to measure the medicinal properties of new medications which is principally popular in emerging areas. In our article, in terms of vertex degrees of molecular graph of drugs, we determined the well popular topological indices of certain molecular graphs which are widely appear in drug structures as an application for pharmacy engineering.

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