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Expected values of various degree-based graph invariants of Azythromycin

M.C. Shanmukha[a,*], A. Usha[b], G.S. Pallavi[c]

[a]Department of Mathematics, PES Institute of Technology and Management, Shivamogga-577204, India.

[b]Department of Mathematics, Alliance School of Applied Mathematics, Bangalore-562106, India.

[c]Department of Mathematics, Bapuji Institute of Engineering & Technology, Davanagere-577004, India.

Abstract

The greatest innovation of the 20^{th} century is the launch of antibiotics into the clinical use. It helps in treating infectious diseases caused by bacteria and in addition to this, it is used in the cancer treatment, organ transplant and open-heart surgery. This work focusses on a miracle antibiotic, Azithromycin which is used in several diseases caused by bacteria. The detailed study on this compound is discussed in the forthcoming sections. This article pinpoints on computing various degree-based topological indices for Azithromycin followed by the numerical representation of the considered indices in tabulated form for better understanding.

Keywords: Chemical graph theory, topological indices, Azithromycin.

2020 MSC: 05C07, 05C10, 05C90.

1. Introduction

A 15-membered macrocyclic lactone ring attached to sugar moieties is a subclass of macrolides. This is referred to as the antibiotic called Azithromycin (Figure 1) [1, 2]. This macrolide is used in the treatment of bacteria causing infection related to respiratory, skin, ear, eye and sexually transmitted diseases. It is not restricted to the infections mentioned above. Azithromycin has to be consumed only when the doctor prescribes it based on the examination of the patient and his/her ailment. It can harm the system if consumed overdose leading to poison. Such situations are to be looked in immediately by consulting the physician. There are various side effects on the consumption of azithromycin. Overdose or frequent usage of this drug can cause damage to liver. Also, the patients should not consume this drug if they are allergic to clarithromycin, erythromycin, or telithromycin. The patient who has the history of jaundice and kidney related issues is not advised to use azithromycin. This drug is not expected to harm an unborn baby. It means this drug may be consumed by the patient who is expecting a child or who is planning to conceive. The studies also show that it does not cause any harm to the baby through the nursing mother. For the treatment of chlamydia trachomatis, the first azalide antibiotic used was Azithromycin [3]. It was approved for a single dose treatment for nongonococcal urethritis and cervicitis. Apart from this,

*Corresponding author

Email addresses: mcshanmukha@gmail.com (M.C. Shanmukha), usha.arcot@alliance.edu.in (A. Usha), pallavipallu0316@gmail.com (G.S. Pallavi)

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it is used in treating the infections caused in the respiratory tract and skin. James [4] found that the C. trachomatis was the most common disease in 1990 in the United States. It was the cause for nongonococcal urethritis and epididymitis in men below 35 years of age. In women, it causes pelvic inflammatory disease (PID). For the treatment of genital infections, despite mild side effects, tetracycline was administered orally. Tetracycline was prescribed for pregnant women has shown that it was not so tolerant in these women which was effective against C.trachomatis infection than chlamydial infections. As a substitution to tetracycline, erythromycin was used in pregnant women as tetracycline was harmful not only to the mother but also to the foetus. Bacterial protein synthesis is inhibited through binding to 50S ribosomal subunit of susceptible organisms by producing antibacterial effects by Azithromycin which is like erythromycin. Azithromycin is noteworthy because of its unique cellular kinetics that has rapid and extensive penetration into intracellular and interstitial tissue compartments. The absorption of azithromycin is more familiar than erythromycin, that produces higher tissue concentrations [5, 6, 7].

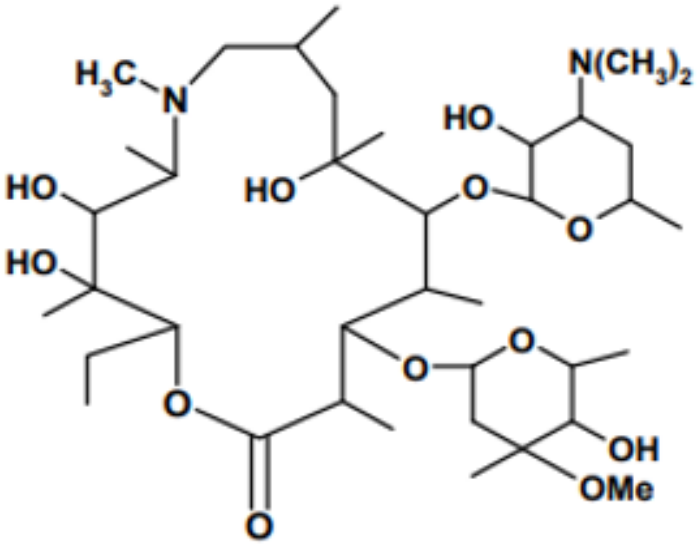

Figure 1: The molecular structure of Azithromycin.

In chemical graph theory a mathematical formula that can be applied to any graph refers to a topological index or numerical invariant [8, 9, 10]. In the literature, various topological indices discussed based on degree and its neighborhood degree for numerous graph structures, helps in analysing physico-chemical properties of molecule [12, 11]. This tool is very efficient as it is cost effective and requires less time.

In the present scenario, numerical invariants play remarkable role in the investigation of physico-chemical properties, biological activities of chemical compounds through QSAR/QSPR/QSTR studies [13, 14, 16, 15, 17, 18, 19].

The drastic growth of the studies on topological theory widened the thinking of chemists about the chemical behaviour of the compounds by examining its molecular graph. The indices help the chemists to understand its characteristics, which help in the applications related to bioinformatics and proteomics. The study of topological indices help the researchers work on the compounds and its chemical network making it possible to elaborate their inquests related to drugs, medicine, medical research, and experimental science in the QSAR/QSPR analysis [20, 21]. The topological indices are computed assuming the atoms as vertices and their bonds as edges. Let $G = (V, E)$ be a simple graph with V and E denoting the vertices and edges respectively. For graph terminologies and notations refer [22, 23, 24].

Gutman and Trinajstic [25, 26] proposed first and second Zagreb indices and are defined as follows

$$M_1(G) = \sum_{v\omega \in E(G)} (d_v + d_\omega) \tag{1.1}$$

$$M_2(G) = \sum_{v\omega \in E(G)} (d_v \times d_\omega) \tag{1.2}$$

In the year 1975, Milan Randic [27] proposed the classic index namely, Randic index and is defined as

$$R(G) = \sum_{v\omega \in E(G)} \frac{1}{\sqrt{(d_v \times d_\omega)}}$$

In 1998, Bollobas et al. [28] proposed the general Randic index and is defined as

$$R_\alpha(G) = \sum_{v\omega \in E(G)} (d_v \times d_\omega)^\alpha \tag{1.3}$$

Fajtlowicz proposed Harmonic index [29] and is defined as

$$H(G) = \sum_{v\omega \in E(G)} \frac{2}{(d_v + d_\omega)} \tag{1.4}$$

Zhou et al. [30] proposed Sum-Connectivity index and is defined as

$$SC(G) = \sum_{v\omega \in E(G)} \frac{1}{\sqrt{(d_v + d_\omega)}} \tag{1.5}$$

A novel molecular descriptor called the SS index is proposed by Weidong Zhao et al.[31] and is stated as

$$SS(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_v \times d_\omega}{d_v + d_\omega}} \tag{1.6}$$

Furtula et al. [32] proposed Forgotten index and is defined as

$$F(G) = \sum_{v\omega \in E(G)} (d_v)^2 + (d_\omega)^2 \tag{1.7}$$

Estrada et al. [33] proposed Atom-bond connectivity index and is defined as

$$ABC(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_v + d_\omega - 2}{d_v \times d_\omega}} \tag{1.8}$$

Vukicevic et al., [34] proposed geometric-arithmetic index and is defined as

$$GA(G) = \sum_{v\omega \in E(G)} \frac{2\sqrt{d_v \times d_\omega}}{d_v + d_\omega} \tag{1.9}$$

Usha et al. [35] proposed geometric-harmonic index and is defined as

$$GH(G) = \sum_{v\omega \in E(G)} \frac{(d_v + d_\omega)(\sqrt{d_v \times d_\omega})}{2} \tag{1.10}$$

Recently, Gutman [36] formulated Sombor index and is defined as

$$SO(G) = \sum_{\nu\omega \in E(G)} \sqrt{(d_\nu)^2 + (d_\omega)^2} \tag{1.11}$$

The fourth Atom-bond connectivity index proposed by Ghorbani et al. [37] and is defined as

$$ABC_4(G) = \sum_{\nu\omega \in E(G)} \sqrt{\frac{S_\nu + S_\omega - 2}{S_\nu \times S_\omega}} \tag{1.12}$$

The fifth geometric-arithmetic index was defined by Graovac et al. [38] and is defined as

$$GA_5(G) = \sum_{\nu\omega \in E(G)} \frac{2\sqrt{S_\nu \times S_\omega}}{S_\nu + S_\omega} \tag{1.13}$$

2. Methodology

Initially, the molecular structure of Azithromycin is modelled as molecular graph and vertex and edge partitions are determined. The familiar degree-based topological indices are computed for the above said molecular graph. In this procedure, the methods used are vertex partition, edge partition and combinatorial computing.

3. Results for molecular graph of Azithromycin

From Figure 2, the details of degrees of vertices and their edges are tabulated in Table 1 for the molecular graph of Azithromycin.

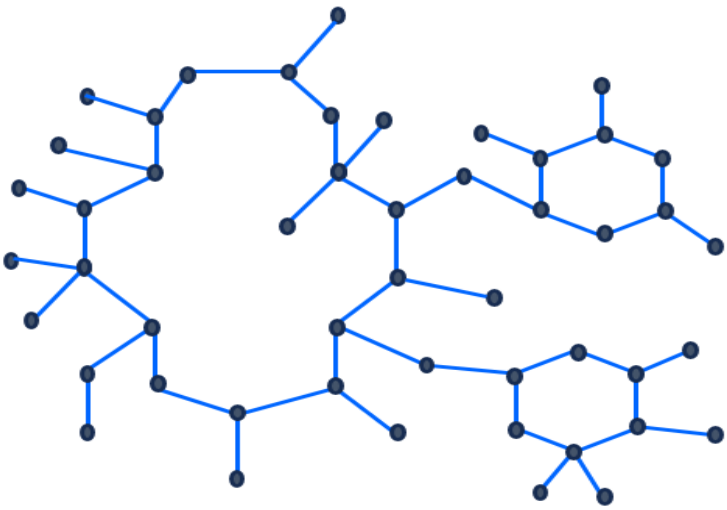

Figure 2: The molecular graph of Azithromycin.

Theorem 3.1. Consider a molecular graph G for Azithromycin, then

$$M_1(G) = 260.$$

Table 1: The edge partition of molecular graph of Azithromycin based on degrees of the end vertices of each edge

(d_v, d_ω) where $v\omega \in E(G)$	No. of edges
(1,2)	1
(1,3)	12
(1,4)	6
(2,3)	17
(2,4)	2
(3,3)	9
(3,4)	4

Table 2: The edge partition of molecular graph of Azithromycin based on neighbour degrees of the end vertices of each edge

(S_v, S_ω) where $v\omega \in E(G)$	No. of edges
(2,4)	1
(3,5)	2
(3,6)	4
(3,7)	4
(3,8)	2
(4,7)	4
(4,8)	3
(5,6)	3
(5,7)	1
(6,6)	6
(6,7)	6
(6,8)	3
(6,9)	1
(7,7)	3
(7,8)	4
(7,9)	2
(8,8)	2

Proof. From equation (1.1) and Table 1, the $M_1(G)$ for Azithromycin, we get

$$\begin{aligned} M_1(G) &= \sum_{v\omega \in E(G)} (d_v + d_\omega) \\ &= 1(1+2) + 12(1+3) + 6(1+4) + 17(2+3) + 2(2+4) + 9(3+3) + 4(3+4) \\ M_1(G) &= 260. \end{aligned}$$

□

Theorem 3.2. Consider a molecular graph G for Azithromycin, then

$$M_2(G) = 309.$$

Proof. From equation (1.2) and Table 1, the $M_2(G)$ for Azithromycin, we get

$$\begin{aligned} M_2(G) &= \sum_{v\omega \in E(G)} (d_v \times d_\omega) \\ &= 1(1\times 2) + 12(1\times 3) + 6(1\times 4) + 17(2\times 3) + 2(2\times 4) + 9(3\times 3) + 4(3\times 4) \\ M_2(G) &= 309. \end{aligned}$$

□

Theorem 3.3. Consider a molecular graph G for Azithromycin, then

$$R_\alpha(G) = 22.44.$$

Proof. From equation (1.3) and Table 1, the $R_\alpha(G)$ for Azithromycin, we get

$$\begin{aligned} R_\alpha(G) &= \sum_{v\omega\in E(G)} (d_v \times d_\omega)^\alpha, \quad \alpha = -\frac{1}{2} \\ &= 1(1\times 2)^\alpha + 12(1\times 3)^\alpha + 6(1\times 4)^\alpha + 17(2\times 3)^\alpha + 2(2\times 4)^\alpha + 9(3\times 3)^\alpha + 4(3\times 4)^\alpha \\ R_\alpha(G) &= 22.44. \end{aligned}$$

□

Theorem 3.4. Consider a molecular graph G for Azithromycin, then

$$H(G) = 20.676.$$

Proof. From equation (1.4) and Table 1, the $H(G)$ for Azithromycin, we get

$$\begin{aligned} H(G) &= \sum_{v\omega\in E(G)} \frac{2}{(d_v + d_\omega)} \\ &= 1\left\{\frac{2}{(1+2)}\right\} + 12\left\{\frac{2}{(1+3)}\right\} + 6\left\{\frac{2}{(1+4)}\right\} 1 + 17\left\{\frac{2}{(2+3)}\right\} + 2\left\{\frac{2}{(2+4)}\right\} \\ &+ 9\left\{\frac{2}{(3+3)}\right\} + 4\left\{\frac{2}{(3+4)}\right\} \\ H(G) &= 20.676. \end{aligned}$$

□

Theorem 3.5. Consider a molecular graph G for Azithromycin, then

$$SC(G) = 22.866.$$

Proof. From equation (1.5) and Table 1, the $SC(G)$ for Azithromycin, we get

$$\begin{aligned} SC(G) &= \sum_{v\omega\in E(G)} \frac{1}{\sqrt{(d_v + d_\omega)}} \\ &= 1\left\{\frac{1}{\sqrt{(1+2)}}\right\} + 12\left\{\frac{1}{\sqrt{(1+3)}}\right\} + 6\left\{\frac{1}{\sqrt{(1+4)}}\right\} 1 + 17\left\{\frac{1}{\sqrt{(2+3)}}\right\} \\ &+ 2\left\{\frac{1}{\sqrt{(2+4)}}\right\} + 9\left\{\frac{1}{\sqrt{(3+3)}}\right\} + 4\left\{\frac{1}{\sqrt{(3+4)}}\right\} \\ SC(G) &= 22.866. \end{aligned}$$

□

Theorem 3.6. Consider a molecular graph G for Azithromycin, then

$$SS(G) = 53.767.$$

Proof. From equation (1.6) and Table 1, the $SS(G)$ for Azithromycin, we get

$$\begin{aligned}
SS(G) &= \sum_{\nu\omega\in E(G)} \sqrt{\frac{(d_\nu \times d_\omega)}{(d_\nu + d_\omega)}} \\
&= 1\left\{\sqrt{\frac{1\times 2}{1+2}}\right\} + 12\left\{\sqrt{\frac{1\times 3}{1+3}}\right\} + 6\left\{\sqrt{\frac{1\times 4}{1+4}}\right\} + 17\left\{\sqrt{\frac{2\times 3}{2+3}}\right\} + 2\left\{\sqrt{\frac{2\times 4}{2+4}}\right\} \\
&+ 9\left\{\sqrt{\frac{3\times 3}{3+3}}\right\} + 4\left\{\sqrt{\frac{3\times 4}{3+4}}\right\} \\
SS(G) &= 53.767.
\end{aligned}$$

□

Theorem 3.7. Consider a molecular graph G for Azithromycin, then

$$F(G) = 750.$$

Proof. From equation (1.7) and Table 1, the forgotten index of molecular graph G for Azithromycin, we get

$$\begin{aligned}
F(G) &= \sum_{\nu\omega\in E(G)} (d_\nu)^2 + (d_\omega)^2 \\
&= 1[(1)^2 + (2)^2] + 12[(1)^2 + (3)^2] + 6[(1)^2 + (4)^2] + 17[(2)^2 + (3)^2] + 2[(2)^2 + (4)^2] \\
&+ 9[(3)^2 + (3)^2] + 4[(3)^2 + (4)^2] \\
F(G) &= 750.
\end{aligned}$$

□

Theorem 3.8. Consider a molecular graph G for Azithromycin, then

$$ABC(G) = 37.79.$$

Proof. From equation (1.8) and Table 1, the $ABC(G)$ for Azithromycin, we get

$$\begin{aligned}
ABC(G) &= \sum_{\nu\omega\in E(G)} \sqrt{\frac{d_\nu + d_\omega - 2}{d_\nu \times d_\omega}} \\
&= (1)\{\sqrt{\frac{1+2-2}{1\times 2}}\} + 12\{\sqrt{\frac{1+3-2}{1\times 3}}\} + 6\{\sqrt{\frac{1+4-2}{1\times 4}}\} + 17\{\sqrt{\frac{2+3-2}{2\times 3}}\} \\
&+ 2\{\sqrt{\frac{2+4-2}{2\times 4}}\} + 9\{\sqrt{\frac{3+3-2}{3\times 3}}\} + 4\{\sqrt{\frac{3+4-2}{3\times 4}}\} \\
ABC(G) &= 37.79.
\end{aligned}$$

□

Theorem 3.9. Consider a molecular graph G for Azithromycin, then

$$GA(G) = 47.636.$$

Proof. From equation (1.9) and Table 1, the $GA(G)$ for Azithromycin, we get

$$\begin{aligned}
GA(G) &= \sum_{v\omega\in E(G)} \frac{2\sqrt{d_v \times d_\omega}}{d_v + d_\omega} \\
&= \{\frac{2(\sqrt{1\times 2})}{(1+2)}\} + 12\{\frac{2(\sqrt{1\times 3})}{(1+3)}\} + 6\{\frac{2(\sqrt{1\times 4})}{(1+4)}\} + 17\{\frac{2(\sqrt{2\times 3})}{(2+3)}\} \\
&+ 2\{\frac{2(\sqrt{2\times 4})}{(2+4)}\} + 9\{\frac{2(\sqrt{3\times 3})}{(3+3)}\} + 4\{\frac{2(\sqrt{3\times 4})}{(3+4)}\} \\
GA(G) &= 47.636.
\end{aligned}$$

□

Theorem 3.10. Consider a molecular graph G for Azithromycin, then

$$GH(G) = 324.262.$$

Proof. From equation (1.10) and Table 1, the GH index of molecular graph G for Azithromycin, we get

$$\begin{aligned}
GH(G) &= \sum_{v\omega\in E(G)} \frac{(d_v + d_\omega)(\sqrt{d_v \times d_\omega})}{2} \\
&= 1\{\frac{(1+2)(\sqrt{1\times 2})}{2}\} + 12\{\frac{(1+3)(\sqrt{1\times 3})}{2}\} + 6\{\frac{(1+4)(\sqrt{1\times 4})}{2}\} \\
&+ 17\{\frac{(2+3)(\sqrt{2\times 3})}{2}\} + 2\{\frac{(2+4)(\sqrt{2\times 4})}{2}\} + 9\{\frac{(3+3)(\sqrt{3\times 3})}{2}\} \\
&+ 4\{\frac{(3+4)(\sqrt{3\times 4})}{2}\} \\
GH(G) &= 324.262.
\end{aligned}$$

□

Theorem 3.11. Consider a molecular graph G for Azithromycin, then

$$SO(G) = 193.344.$$

Proof. From equation (1.11) and Table 1, the Somber index of molecular graph G for Azithromycin, we get

$$\begin{aligned}
SO(G) &= \sum_{v\omega\in E(G)} \sqrt{(d_v)^2 + (d_\omega)^2} \\
&= 1[\sqrt{(1)^2 + (2)^2}] + 12[\sqrt{(1)^2 + (3)^2}] + 6[\sqrt{(1)^2 + (4)^2}] + 17[\sqrt{(2)^2 + (3)^2}] \\
&+ 2[\sqrt{(2)^2 + (4)^2}] + 9[\sqrt{(3)^2 + (3)^2}] + 4[\sqrt{(3)^2 + (4)^2}] \\
SO(G) &= 193.344.
\end{aligned}$$

□

Theorem 3.12. Consider a molecular graph G for Azithromycin, then

$$ABC_4(G) = 27.7962.$$

Proof. From equation (1.12) and Table 2, the $ABC_4(G)$ for Azithromycin, we get

$$\begin{aligned}
ABC_4(G) &= \sum_{\nu\omega\in E(G)} \sqrt{\frac{S_\nu + S_\omega - 2}{S_\nu \times S_\omega}} \\
&= (1)\{\sqrt{\frac{2+4-2}{2\times 4}}\} + 2\{\sqrt{\frac{3+5-2}{3\times 5}}\} + 4\{\sqrt{\frac{3+6-2}{3\times 6}}\} + 4\{\sqrt{\frac{3+7-2}{3\times 7}}\} \\
&+ 2\{\sqrt{\frac{3+8-2}{3\times 8}}\} + 4\{\sqrt{\frac{4+7-2}{4\times 7}}\} + 3\{\sqrt{\frac{4+8-2}{4\times 8}}\} + 3\{\sqrt{\frac{5+6-2}{5\times 6}}\} \\
&+ 1\{\sqrt{\frac{5+7-2}{5\times 7}}\} + 6\{\sqrt{\frac{6+6-2}{6\times 6}}\} + 6\{\sqrt{\frac{6+7-2}{6\times 7}}\} + 3\{\sqrt{\frac{6+8-2}{6\times 8}}\} \\
&+ 1\{\sqrt{\frac{6+9-2}{6\times 9}}\} + 3\{\sqrt{\frac{7+7-2}{7\times 7}}\} + 4\{\sqrt{\frac{7+8-2}{7\times 8}}\} + 2\{\sqrt{\frac{7+9-2}{7\times 9}}\} \\
&+ 2\{\sqrt{\frac{8+8-2}{8\times 8}}\} \\
ABC_4(G) &= 27.7962.
\end{aligned}$$

□

Theorem 3.13. Consider a molecular graph G for Azithromycin, then

$$GA_5(G) = 49.655.$$

Proof. From equation (1.13) and Table 2, the $GA_5(G)$ for Azithromycin, we get

$$\begin{aligned}
GA_5(G) &= \sum_{\nu\omega\in E(G)} \frac{2\sqrt{S_\nu \times S_\omega}}{S_\nu + S_\omega} \\
&= 1\{\frac{2(\sqrt{2\times 4})}{(2+4)}\} + 2\{\frac{2(\sqrt{3\times 5})}{(3+5)}\} + 4\{\frac{2(\sqrt{3\times 6})}{(3+6)}\} + 4\{\frac{2(\sqrt{3\times 7})}{(3+7)}\} + 2\{\frac{2(\sqrt{3\times 8})}{(3+8)}\} \\
&+ 4\{\frac{2(\sqrt{4\times 7})}{(4+7)}\} + 3\{\frac{2(\sqrt{4\times 8})}{(4+8)}\} + 3\{\frac{2(\sqrt{5\times 6})}{(5+6)}\} + 1\{\frac{2(\sqrt{5\times 7})}{(5+7)}\} + 6\{\frac{2(\sqrt{6\times 6})}{(6+6)}\} \\
&+ 6\{\frac{2(\sqrt{6\times 7})}{(6+7)}\} + 3\{\frac{2(\sqrt{6\times 8})}{(6+8)}\} + 1\{\frac{2(\sqrt{6\times 9})}{(6+9)}\} + 3\{\frac{2(\sqrt{7\times 7})}{(7+7)}\} + 4\{\frac{2(\sqrt{7\times 8})}{(7+8)}\} \\
&+ 2\{\frac{2(\sqrt{7\times 9})}{(7+9)}\} + 2\{\frac{2(\sqrt{8\times 8})}{(8+8)}\} \\
GA_5(G) &= 49.655.
\end{aligned}$$

□

4. Comparisons

Table 3: Numerical representation of the computed indices of Azithromycin.

M_1	M_2	R_α	H	SC	SS	F	ABC	GA	GH	SO	ABC_4	GA_5
260	309	22.44	20.676	22.866	53.767	750	37.79	47.636	324.262	193.344	27.796	49.655

Conclusion

Novel antibiotic classes are being discovered frequently in the golden age of antibiotic findings. This is being done by isolation of likely antibiotic-producing organisms from the soil samples. The bio accessibility of azithromycin is 37% whose elimination half life is more than 10-folds compared to other available macrolides. Azithromycin's concentration in tissues is 10 to 100 folds than in the serum. This work focussed on the detailed study of the compound, Azithromycin for which various degree-based topological indices are computed. For more clarity in the variation of these indices, it is tabulated in Table 3. As antibiotics are in great use in our daily life which concentrates on the treatment of bacterial infection, this study may directs the pharmacists/chemists/researchers for further studies in this compound, azithromycin.

Conflict of interest

The authors have no conflict of interest.

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