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Degree-based Numerical Invariants of Amoxicillin

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Abstract

Back in the millennia, the open wounds were being treated using traditional poultices of mould bread before the use of antibiotic-producing microbes in Egypt, Greece, and Serbia. In recent times, the usage of antibiotics has considerably reduced the mortality rate in young children and adults. Amoxicillin is one such antibiotic that is useful in treating bacterial infections, mainly in the ear, eye, nose, and urinary tract. It causes side effects such as loose, watery stools. In this work various degree-based and neighborhood degree-based indices are computed for Amoxicillin.

Keywords: Amoxicillin, bacterial infections, chemical graph theory, topological indices

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

1. Introduction

Amoxicillin is an antibiotic used in treating infection caused by bacteria. It is a penicillin antibiotic. For stomach infections, it is usually mixed with another antibiotic called Biaxin. It is used in treating the infections caused in the ear, throat, nose, and urinary tract. It must be consumed only when the medical practitioner prescribes it after thorough diagnosis. If the patient is allergic to penicillin antibiotic, ampicillin, dicloxacillin and others, liver or kidney disorder, asthma, blood clotting disorder or any other complications then this drug is not advised.

The usage of amoxicillin makes the birth control pills less effective. Amoxycillin usage can cause diarrhea. Amoxicillin's physical properties[1, 2, 3] include its white powdery texture and compatible with citrate. It has sulphurous odour, phosphate, and borate buffers. It is slightly soluble in ethanol, insoluble in fatty oils, Amoxicillin sodium is soluble in water.

In the year 1970's, Amoxicillin was first introduced for oral use in the United Kingdom, and it has gradually taken a broad place in treating the infections caused by bacteria and other diseases. Amoxicillin has been found more effective in treating gram positive bacteria than gram negative bacteria. Several health issues are caused by these bacteria. They are classified based on their structures and appearance after gram

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staining. The process of viewing the bacteria beneath a microscope after they are dyed is called gram staining. Amoxicillin has shown greater efficacy to penicillin and penicillin V in terms of its performance in treating the bacteria.

In the recent years, amoxycillin is reportedly shown remarkable improvements in the treatment of otitis media, tonsillitis and tonsillopharyngitis, throat, pharynx, larynx, bronchi, lungs, urinary tract, skin, and gonorrhea. Recent studies suggest that amoxycillin can be used for patients undergoing prosthetic joint replacements and in dentistry as prophylaxis against bacterial endocarditis.

Human morbidity and mortality were due to infectious diseases (IDs) for many decades till recent times. At present also, IDs contribute to large proportion of death and other disabilities in the world. They are the major threats to public health issues in developing and developed countries. India and Africa are the worst hit every year where children and young adults die because of these IDs.

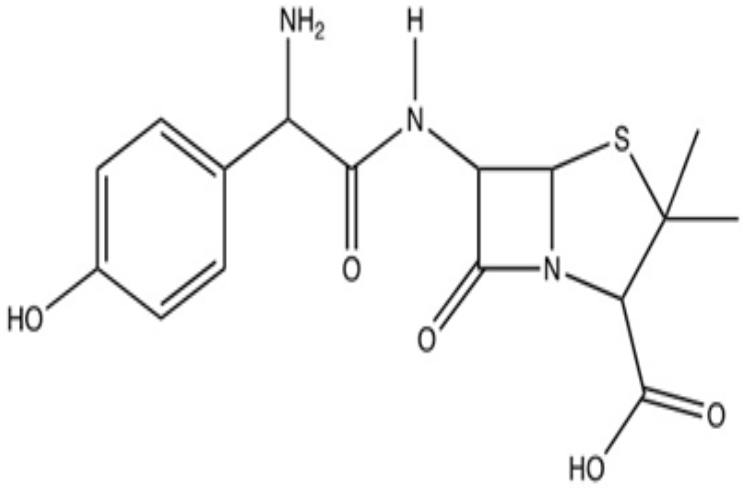

Figure 1: The molecular structure of Amoxicillin.

In 2005, the World Health Organization declared that the leading cause of mortality in children in the world is because of infections, especially acute respiratory infections causing deaths of all ages. The existence and usage of antibiotics have led to the progressive decline of infections leading to deaths. The most important challenge for the medical practitioners is the selection of the appropriate antibiotic based on the diagnosis.

In this work Amoxicillin is considered as a molecular graph for which various topological indices [4, 5, 6, 7] are computed. The topological index is a very helpful tool in chemical graph theory. They are useful in extracting the chemical information of the compound [8, 9, 10, 11, 12, 13] which is applied in drug design and drug delivery in Quantitative Structure Property Relationship (QSPR) studies. There are several topological indices available which are categorized based on degree/neighbor degree/distance. This study concentrates on various indices for which amoxicillin is computed and tabulated as discussed below.

In 2013, Shirdel et al. [14] proposed the first hyper Zagreb index and in 2016, Wei et al. introduced the second hyper-Zagreb index and are defined as follows.

$$HM_1(G) = \sum_{v\omega \in E(G)} (d_v + d_\omega)^2 \tag{1.1}$$

$$HM_2(G) = \sum_{v\omega \in E(G)} (d_v \times d_\omega)^2 \tag{1.2}$$

Kulli [15] proposed the first and the second Gourava indices and are defined as

$$GO_1(G) = \sum_{v\omega \in E(G)} (d_v + d_\omega) + (d_v d_\omega)$$
$$GO_2(G) = \sum_{v\omega \in E(G)} (d_v + d_\omega)(d_v d_\omega)$$

Kulli [16] introduced the first and the second hyper-Gourava indices and are defined as

$$HGO_1(G) = \sum_{v\omega \in E(G)} ((d_v + d_\omega + (d_v d_\omega))^2$$
$$HGO_2(G) = \sum_{v\omega \in E(G)} [(d_v + d_\omega)(d_v d_\omega)]^2$$

Kulli [17] proposed Sum-connectivity Gourava index and is defined as

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

Kulli [17] proposed Product-connectivity Gourava index and is defined as

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

Shanmukha et al. [18] proposed Neighborhood redefined first and second Zagreb indices and are defined as

$$NReZ_1(G) = \sum_{v\omega \in E(G)} \frac{d_v + d_\omega}{d_v d_\omega}$$
$$NReZ_2(G) = \sum_{v\omega \in E(G)} \frac{d_v d_\omega}{d_v + d_\omega}$$

2. Methodology

Initially, the molecular structure of Amoxicillin is modelled as molecular graph, vertex, and edge partitions are determined. The popular 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 Amoxicillin

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

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

$$HM_1(G) = 726.$$

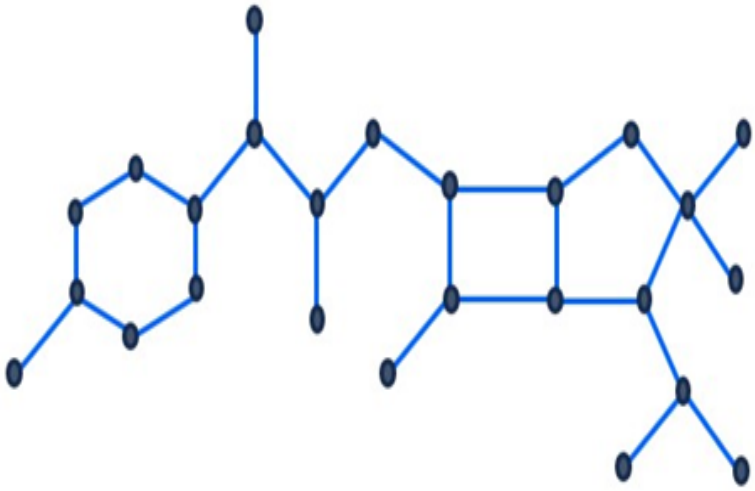

Figure 2: The molecular graph of Amoxicillin.

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

(d_v, d_ω) where $v\omega \in E(G)$	No. of edges
(1, 3)	6
(1, 4)	2
(2, 2)	2
(2, 3)	7
(2, 4)	1
(3, 3)	8
(3, 4)	1

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

(S_v, S_ω) where $v\omega \in E(G)$	No. of edges
(3, 5)	3
(3, 6)	1
(3, 7)	2
(4, 7)	2
(5, 5)	4
(5, 7)	2
(5, 10)	1
(6, 6)	1
(6, 7)	1
(6, 8)	1
(7, 7)	2
(7, 8)	2
(7, 9)	1
(7, 10)	1
(8, 8)	1
(8, 9)	1
(9, 10)	1

Proof. From equation (1.1) and Table 1, the $HM_1(G)$ for Amoxicillin, we get

$$\begin{aligned} HM_1(G) &= \sum_{v\omega\in E(G)} (d_v + d_\omega)^2 \\ &= 6(1+3)^2 + 2(1+4)^2 + 2(2+2)^2 + 7(2+3)^2 + 1(2+4)^2 + 8(3+3)^2 + 1(3+4)^2 \\ HM_1(G) &= 726. \end{aligned}$$

□

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

$$HM_2(G) = 1226.$$

Proof. From equation (1.2) and Table 1, the $HM_2(G)$ for Amoxicillin, we get

$$\begin{aligned} HM_2(G) &= \sum_{v\omega\in E(G)} (d_v \times d_\omega)^2 \\ &= 6(1\times 3)^2 + 2(1\times 4)^2 + 2(2\times 2)^2 + 7(2\times 3)^2 + 1(2\times 4)^2 + 8(3\times 3)^2 + 1(3\times 4)^2 \\ HM_2(G) &= 1226. \end{aligned}$$

□

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

$$GO_1(G) = 306.$$

Proof. From equation (1.3) and Table 1, the $GO_1(G)$ for Amoxicillin, we get

$$\begin{aligned} GO_1(G) &= \sum_{v\omega\in E(G)} (d_v + d_\omega + d_v d_\omega) \\ &= 6(1+3+1\times 3) + 2(1+4+1\times 4) + 2(2+2+2\times 2) + 7(2+3+2\times 3) + 1(2+4+2\times 4) \\ &+ 8(3+3+3\times 3) + 1(3+4+3\times 4) \\ GO_1(G) &= 306. \end{aligned}$$

□

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

$$GO_2(G) = 918.$$

Proof. From equation (1.4) and Table 1, the $GO_2(G)$ for Amoxicillin, we get

$$\begin{aligned} GO_2(G) &= \sum_{v\omega\in E(G)} (d_v + d_\omega)(d_v d_\omega) \\ &= 6(1+3)(1\times 3) + 2(1+4)(1\times 4) + 2(2+2)(2\times 2) + 7(2+3)(2\times 3) + 1(2+4)(2\times 4) \\ &+ 8(3+3)(3\times 3) + 1(3+4)(3\times 4) \\ GO_2(G) &= 918. \end{aligned}$$

□

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

$$HGO_1(G) = 3788.$$

Proof. From equation (1.3) and Table 1, the $HGO_1(G)$ for Amoxicillin, we get

$$HGO_1(G) = \sum_{\nu\omega\in E(G)} (d_\nu + d_\omega + d_\nu d_\omega)^2$$
$$= 6(1+3+1\times 3)^2 + 2(1+4+1\times 4)^2 + 2(2+2+2\times 2)^2 + 7(2+3+2\times 3)^2 + 1(2+4+2\times 4)^2$$
$$+ 8(3+3+3\times 3)^2 + 1(3+4+3\times 4)^2$$
$$HGO_1(G) = 3788.$$

□

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

$$HGO_2(G) = 41164.$$

Proof. From equation (1.4) and Table 1, the $HGO_2(G)$ for Amoxicillin, we get

$$HGO_2(G) = \sum_{\nu\omega\in E(G)} ((d_\nu + d_\omega)(d_\nu d_\omega))^2$$
$$= 6[(1+3)(1\times 3)]^2 + 2[(1+4)(1\times 4)]^2 + 2[(2+2)(2\times 2)]^2 + 7[(2+3)(2\times 3)]^2 + 1[(2+4)(2\times 4)]^2$$
$$+ 8[(3+3)(3\times 3)]^2 + 1[(3+4)(3\times 4)]^2$$
$$HGO_2(G) = 41164.$$

□

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

$$SGO(G) = 8.314408.$$

Proof. From equation (1.7) and Table 1, the SGO for Amoxicillin, we get

$$SGO(G) = \sum_{\nu\omega\in E(G)} \frac{1}{\sqrt{(d_\nu + d_\omega) + (d_\nu d_\omega)}}$$
$$= 6[\frac{1}{\sqrt{1+3+(1\times 3)}}] + 2[\frac{1}{\sqrt{1+4+(1\times 4)}}] + 2[\frac{1}{\sqrt{2+2+(2\times 2)}}] + 7[\frac{1}{\sqrt{2+3+(2\times 3)}}]$$
$$+ 1[\frac{1}{\sqrt{2+4+(2\times 4)}}] + 8[\frac{1}{\sqrt{3+3+(3\times 3)}}] + 1[\frac{1}{\sqrt{3+4+(3\times 4)}}]$$
$$SGO(G) = 8.314408.$$

□

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

$$PGO(G) = 5.2994.$$

Proof. From equation (1.7) and Table 1, the PGO for Amoxicillin, we get

$$PGO(G) = \sum_{\nu\omega\in E(G)} \frac{1}{\sqrt{(d_\nu + d_\omega)(d_\nu d_\omega)}}$$
$$= 6[\frac{1}{\sqrt{(1+3)(1\times 3)}}] + 2[\frac{1}{\sqrt{(1+4)(1\times 4)}}] + 2[\frac{1}{\sqrt{(2+2)(2\times 2)}}]$$
$$+ 7[\sqrt{\frac{1}{(2+3)(2\times 3)}}] + 1[\sqrt{\frac{1}{(2+4)(2\times 4)}}] + 8[\sqrt{\frac{1}{(3+3)(3\times 3)}}] + 1[\frac{1}{\sqrt{(3+4)(3\times 4)}}]$$
$$PGO(G) = 5.2994.$$

□

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

$$NReZ_1(G) = 9.65949.$$

Proof. From equation (1.4) and Table 1, the $NReZ_1(G)$ for Amoxicillin, we get

$$\begin{aligned}
NReZ_1(G) &= \sum_{\nu\omega\in E(G)} \frac{d_\nu + d_\omega}{d_\nu d_\omega} \\
&= 3[\frac{3+5}{3\times 5}] + 1[\frac{3+6}{3\times 6}] + 2[\frac{3+7}{3\times 7}] + 2[\frac{4+7}{4\times 7}] + 4[\frac{5+5}{5\times 5}] + 2[\frac{5+7}{5\times 7}] + 1[\frac{5+10}{5\times 10}] + 1[\frac{6+6}{6\times 6}] + 1[\frac{6+7}{6\times 7}] \\
&+ 1[\frac{6+8}{6\times 8}] + 2[\frac{7+7}{7\times 7}] + 2[\frac{7+8}{7\times 8}] + 1[\frac{7+9}{7\times 9}] + 1[\frac{7+10}{7\times 10}] + 1[\frac{8+8}{8\times 8}] + 1[\frac{8+9}{8\times 9}] + 1[\frac{9+10}{9\times 10}] \\
NReZ_1(G) &= 9.65949.
\end{aligned}$$

□

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

$$NReZ_2(G) = 76.0136.$$

Proof. From equation (1.4) and Table 1, the $NReZ_2(G)$ for Amoxicillin, we get

$$\begin{aligned}
NReZ_2(G) &= \sum_{\nu\omega\in E(G)} \frac{d_\nu d_\omega}{d_\nu + d_\omega} \\
&= 3[\frac{3\times 5}{3+5}] + 1[\frac{3\times 6}{3+6}] + 2[\frac{3\times 7}{3+7}] + 2[\frac{4\times 7}{4+7}] + 4[\frac{5\times 5}{5+5}] + 2[\frac{5\times 7}{5+7}] + 1[\frac{5\times 10}{5+10}] + 1[\frac{6\times 6}{6+6}] + 1[\frac{6\times 7}{6+7}] + 1[\frac{6\times 8}{6+8}] \\
&+ 2[\frac{7\times 7}{7+7}] + 2[\frac{7\times 8}{7+8}] + 1[\frac{7\times 9}{7+9}] + 1[\frac{7\times 10}{7+10}] + 1[\frac{8\times 8}{8+8}] + 1[\frac{8\times 9}{8+9}] + 1[\frac{9\times 10}{9+10}] \\
NReZ_2(G) &= 76.0136.
\end{aligned}$$

□

4. Comparisons

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

HM_1	HM_2	GO_1	GO_2	HGO_1	HGO_2	SGO	PGO	$NeRZ_1$	$NeRZ_2$
726	1226	306	918	3788	41164	8.314408	5.2994	9.65949	76.0136

Conclusion

The bactericidal amoxicillin fights against vulnerable micro-organisms through the inhibition of biosynthesis during bacterial multiplications. Because of its significant properties of solubility and concentration, it is very effective in treating bacterial infections. This study concentrates on the computation of degree-based and neighborhood degree-based molecular descriptors of amoxicillin. As the considered compound is very familiar in today's clinical medicine, this work will be useful for chemists/researchers/pharmacists in their further studies of the compound.

Conflict of interest

The authors have no conflict of interest.

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