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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

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 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.

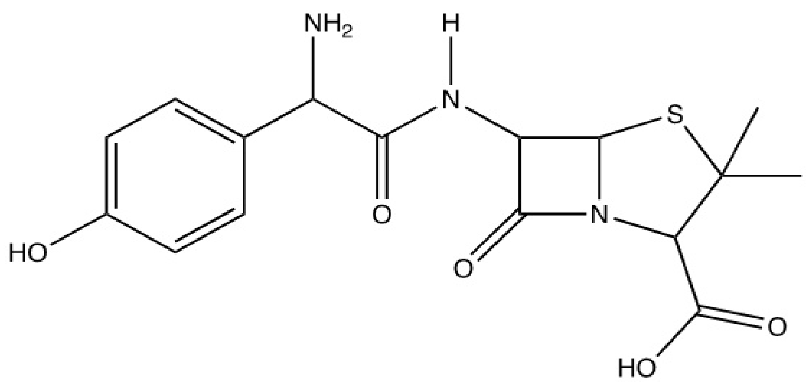


Figure 1: The molecular structure of Amoxicillin.

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 [4-7] 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 [8-13] 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.

$$HM_1(G) = \sum_{vw \in E(G)} (d_v + d_w)^2 \qquad (1)$$

$$HM_2(G) = \sum_{vw \in E(G)} (d_v d_w)^2 \qquad (2)$$

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

$$GO_1(G) = \sum_{vw \in E(G)} (d_v + d_w + d_v d_w) \quad (3)$$

$$GO_2(G) = \sum_{vw \in E(G)} (d_v + d_w) d_v d_w \quad (4)$$

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

$$HGO_1(G) = \sum_{vw \in E(G)} (d_v + d_w + d_v d_w)^2 \quad (5)$$

$$HGO_2(G) = \sum_{vw \in E(G)} [(d_v + d_w) d_v d_w]^2 \quad (6)$$

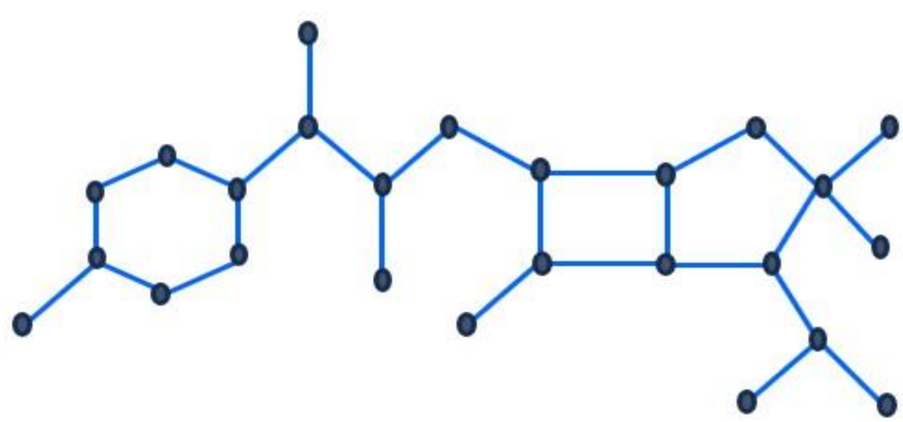
Kulli [17] proposed Sum-Connectivity Gourava index and is defined as

$$SGO(G) = \sum_{vw \in E(G)} \frac{1}{\sqrt{(d_v + d_w + d_v d_w)}} \quad (7)$$

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

$$PGO(G) = \sum_{vw \in E(G)} \sqrt{(d_v + d_w) d_v d_w} \quad (8)$$

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



$$\mathrm{NRe\,Z}_1(G) = \sum_{vw \in E(G)} \frac{d_v + d_w}{d_v d_w} \quad (9)$$

$$\mathrm{NRe\,Z}_2(G) = \sum_{vw \in E(G)} \frac{d_v d_w}{d_v + d_w} \quad (10)$$

2 METHODOLOGY

Figure 2: The molecular graph of Amoxicillin.

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 inTable 1 and Table 2 for the molecular graph of Amoxicillin.

Table 1: The edge partition of molecular graph of Amoxicillin based on degreesof 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

Theorem 3.1. Consider a molecular graph of Amoxicillin, then

$$HM_1(G) = 726$$

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

$$HM_1(G) = \sum_{vw \in E(G)} (d_v + d_w)^2$$
$$= 6(1+3)^2 + 2(1+4)^2 + 2(2+2)^2 + 7(2+3)^2 + 1(2+4)^2 + 8(3+3)^2 + 1(3+4)^2$$
$$HM_1(G) = 726$$

Theorem 3.2. Consider a molecular graph of Amoxicillin, then

$$HM_2(G) = 1226$$

Proof. From equation 2 and Table 1, the $HM_2(G)$ for Amoxicillin is

$$HM_2(G) = \sum_{vw \in E(G)} (d_v \times d_w)^2$$
$$= 6(1\times 3)^2 + 2(1\times 4)^2 + 2(2\times 2)^2 + 7(2\times 3)^2 + 1(2\times 4)^2 + 8(3\times 3)^2 + 1(3\times 4)^2$$
$$HM_2(G) = 1226$$

Theorem 3.3. Consider a molecular graph of Amoxicillin, then

$$GO_1(G) = 306$$

Proof. From equation 3 and Table 1, the $GO_1(G)$ for Amoxicillin is

$$GO_1(G) = \sum_{vw \in E(G)} (d_v + d_w + d_v d_w)$$
$$= 6(1+3+1\times 3) + 2(1+4+1\times 4) + 2(2+2+2\times 2) + 7(2+3+2\times 3)$$
$$+1(2+4+2\times 4) + 8(3+3+3\times 3) + 1(3+4+3\times 4)$$
$$GO_1(G) = 306$$

Theorem 3.4. Consider a molecular graph of Amoxicillin, then

$$GO_2(G) = 918$$

Proof. From equation 4 and Table 1, the $GO_2(G)$ for Amoxicillin is

$$\begin{aligned} GO_2(G) &= \sum_{vw \in E(G)} (d_v + d_w)\, d_v d_w \\ &= 6(1+3)(1\times 3) + 2(1+4)(1\times 4) + 2(2+2)(2\times 2) + 7(2+3)(2\times 3) \\ &\quad +1(2+4)(2\times 4) + 8(3+3)(3\times 3) + 1(3+4)(3\times 4) \\ GO_2(G) &= 918 \end{aligned}$$

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

$$HGO_1(G) = 3788$$

Proof. From equation 5 and Table 1, the $HG0_1(G)$ for Amoxicillin is

$$\begin{aligned} HGO_1(G) &= \sum_{vw \in E(G)} (d_v + d_w + d_v d_w)^2 \\ &= 6(1+3+1\times 3)^2 + 2(1+4+1\times 4)^2 + 2(2+2+2\times 2)^2 + 7(2+3+2\times 3)^2 \\ &\quad +1(2+4+2\times 4)^2 + 8(3+3+3\times 3)^2 + 1(3+4+3\times 4)^2 \\ HGO_1(G) &= 3788 \end{aligned}$$

Theorem 3.6. Consider a molecular graph of Amoxicillin, then

$$HGO_2(G) = 41164$$

Proof. From equation 6 and Table 1, the $HG0_2(G)$ for Amoxicillin is

$$HGO_2(G) = \sum_{vw \in E(G)} [(d_v + d_w) d_v d_w]^2$$
$$= 6[(1+3)(1\times 3)]^2 + 2[(1+4)(1\times 4)]^2 + 2[(2+2)(2\times 2)]^2 + 7[(2+3)(2\times 3)]^2$$
$$+1[(2+4)(2\times 4)]^2 + 8[(3+3)(3\times 3)]^2 + 1[(3+4)(3\times 4)]^2$$
$$HGO_2(G) = 41164$$

Theorem 3.7. Consider a molecular graph of Amoxicillin, then

$$SGO(G) = 8.314408$$

Proof. From equation 7 and Table 1, the $SG0(G)$ for Amoxicillin is

$$SGO(G) = \sum_{vw \in E(G)} \frac{1}{\sqrt{(d_v + d_w + d_v d_w)}}$$
$$= 6\frac{1}{\sqrt{1+3+(1\times 3)}} + 2\frac{1}{\sqrt{1+4+(1\times 4)}} + 2\frac{1}{\sqrt{2+2+(2\times 2)}} + 7\frac{1}{\sqrt{2+3+(2\times 3)}}$$
$$+1\frac{1}{\sqrt{2+4+(2\times 4)}} + 8\frac{1}{\sqrt{3+3+(3\times 3)}} + 1\frac{1}{\sqrt{3+4+(3\times 4)}}$$
$$SGO(G) = 8.314408$$

Theorem 3.8. Consider a molecular graph of Amoxicillin, then

$$PGO(G) = 150.9505$$

Proof. From equation 8 and Table 1, the $\mathrm{PGO}(G)$ for Amoxicillin is

$$PGO(G) = \sum_{vw \in E(G)} \sqrt{(d_v + d_w) d_v d_w}$$
$$= 6\sqrt{(1+3)(1\times 3)} + 2\sqrt{(1+4)(1\times 4)} + 2\sqrt{(2+2)(2\times 2)} + 7\sqrt{(2+3)(2\times 3)}$$
$$+1\sqrt{(2+4)(2\times 4)} + 8\sqrt{(3+3)(3\times 3)} + 1\sqrt{(3+4)(3\times 4)}$$
$$PGO(G) = 150.9505$$

Theorem 3.9. Consider a molecular graph of Amoxicillin, then

$$\mathrm{NRe\,Z}_1(G) = 9.65949$$

Proof. From equation 9 and Table 2, the $\mathrm{NRe\,Z}_1(G)$ for Amoxicillin is

$$\mathrm{NRe\,Z}_1(G) = \sum_{vw \in E(G)} \frac{d_v(u) + d_w(v)}{d_v(u) \cdot d_w(v)}$$

$$= 3\left(\frac{3+5}{3\times5}\right)+1\left(\frac{3+6}{3\times6}\right)+2\left(\frac{3+7}{3\times7}\right)+2\left(\frac{4+7}{4\times7}\right)+4\left(\frac{5+5}{5\times5}\right)+2\left(\frac{5+7}{5\times7}\right)$$
$$+1\left(\frac{5+10}{5\times10}\right)+1\left(\frac{6+6}{6\times6}\right)+1\left(\frac{6+7}{6\times7}\right)+1\left(\frac{6+8}{6\times8}\right)+2\left(\frac{7+7}{7\times7}\right)+2\left(\frac{7+8}{7\times8}\right)$$
$$+1\left(\frac{7+9}{7\times9}\right)+1\left(\frac{7+10}{7\times10}\right)+1\left(\frac{8+8}{8\times8}\right)+1\left(\frac{8+9}{8\times9}\right)+1\left(\frac{9+10}{9\times10}\right)$$
$$\mathrm{NReZ}_1(G) = 9.65949$$

Theorem 3.10. *Consider a molecular graph of* Amoxicillin, *then*

$$\mathrm{NReZ}_2(G) = 76.0136$$

Proof. From equation 10 and Table 2, the $\mathrm{NReZ}_2(G)$ for Amoxicillin is

$$\mathrm{NReZ}_2(G) = \sum_{vw\in E(G)} \frac{d_v(u)\cdot d_w(v)}{d_v(u)+d_w(v)}$$
$$= 3\left(\frac{3\times5}{3+5}\right)+1\left(\frac{3\times6}{3+6}\right)+2\left(\frac{3\times7}{3+7}\right)+2\left(\frac{4\times7}{4+7}\right)+4\left(\frac{5\times5}{5+5}\right)+2\left(\frac{5\times7}{5+7}\right)$$
$$+1\left(\frac{5\times10}{5+10}\right)+1\left(\frac{6\times6}{6+6}\right)+1\left(\frac{6\times7}{6+7}\right)+1\left(\frac{6\times8}{6+8}\right)+2\left(\frac{7\times7}{7+7}\right)+2\left(\frac{7\times8}{7+8}\right)$$
$$+1\left(\frac{7\times9}{7+9}\right)+1\left(\frac{7\times10}{7+10}\right)+1\left(\frac{8\times8}{8+8}\right)+1\left(\frac{8\times9}{8+9}\right)+1\left(\frac{9\times10}{9+10}\right)$$
$$\mathrm{NReZ}_2(G) = 76.0136$$

4 COMPARISONS

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

HM_1	HM_2	GO_1	GO_2	HGO_1	HGO_2	SGO	PGO	$NReZ_1$	$NReZ_2$
726	1226	306	918	3788	41164	8.314408	150.9505	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.

REFERENCES

[1] Simar Preet Kaur, Rekha Rao, Sanju Nanda, Amoxicillin: A Broad-Spectrum Antibiotic (2011), International Journal of Pharmacy and Pharmaceutical Sciences, 3(3).
[2] Mathew I Hutchings, Andrew W Truman, Barrie Wilkinson, Antibiotics: past, present and future, Current Opinion in Microbiology (2019), https://doi.org/10.1016/j.mib.2019.10.008
[3] Brogden RN, Heel RC, Speight TM, Avery GS. Amoxicillin injectable: a review of its antibacterial spectrum, pharmacokinetics, and therapeutic use. Drugs 1979; 18(3): 169-184.
[4] R. Todeschini, and V. Consonni, Handbook of Molecular Descriptors, Wiley- VCH, Weinheim, 2000.
W. Gao, M.R. Farahani, M.K. Jamil, and M.K. Siddiqui, The Redefined First, Second and Third Zagreb Indices of Titania Nanotubes TiO2[m; n], The Open Biotechnology Journal, 10(2016), 272-277.
[5] M. Randic, Novel molecular descriptor for structure-property studies, Chemical Physics Letters, 211(1993), 478–483.
[6] H. Wiener, Structural determination of paraffin boiling points, Journal of the American Chemical Society, 69(1947),17–20.
[7] Shanmukha, M. C., Usha, A., Praveen, B. M., & Douhadji, A. (2022). Degree- based molecular descriptors and QSPR analysis of breast cancer drugs. Journal of Mathematics, 2022, 1-13.
[8] Zhang, X., Reddy, H. G., Usha, A., Shanmukha, M. C., Reza Farahani, M., & Alaeiyan, M. (2022). A study on anti-malaria drugs using degree-based topo- logical indices through QSPR analysis.
[9] Shanmukha, M. C., Ismail, R., Gowtham, K. J., Usha, A., Azeem, M., & Al- Sabri, E. H. A. (2023). Chemical applicability and computation of K-Banhatti indices for benzenoid hydrocarbons and triazine-based covalent organic frame- works. Scientific Reports, 13(1), 17743.
[10] E. Estrada E, E. Uriarte, Recent advances on the role of topological indices in drug discovery research, Curr Med Chem., 8(13) (2001), 1573-88. Doi: 10.2174/0929867013371923.
[11] F. Harary, Graph Theory, Addison-Wesely, Reading Mass, 1969.
[12] V.R. Kulli, College Graph Theory, Vishwa Int. Publ., Gulbarga, India, 2012.
[13] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL. 1992.
[14] G.H. Shirdel, H. Rezapour and A.M. Sayadi, The hyper-Zagreb index of graph operations. Iran. J. Math. Chem. 4 (2013), 2, 213–220.
[15] V. R.Kulli, the Gourava indices and coindices of graphs, Annals of Pure and Applied Mathematics(2017), 14(1).
[16] V.R. Kulli, On hyper-Gourava indices and co indices, International Journal of Mathematical Archive (2017), 8(12).
[17] V. R. Kulli, Sum and Product Connectivity Gourava domination indices of Graphs (2023), 11(4).
[18] M.C. Shanmukha, N.S. Basavarajappa, A. Usha and K.C. Shilpa, Novel Neighbourhood redefined First and Second Zagreb indices on Carborundum Structures, Journal of Applied Mathematics and Computing, 2020, 1-14. DOI: 10.1007/s12190-020-01435-3.