TOPOLOGICAL INDICIES OF CINOXACIN

J Janet Sheeba[1], M Peter[2], P Mahimai Raj[3], T Shiba Neenu[4], S Roseline Mary[5]

Article History: Received: 29.05.2023 **Revised:** 24.06.2023 **Accepted:** 20.07.2023

Abstract

Graph theory has provided chemists with a variety of useful tools, such as topological indices. A topological index Top(G) of a graph G is a number with the property that for every graph H isomorphic to G, Top(H) = Top(G). In this paper, we compute ABC index, ABC_4 index, Randic connectivity index, sum connectivity index, GA index, GA_5 index, first Zagreb index, second Zagreb index, augmented Zagreb index, harmonic index and hyper Zagreb index of Cinoxacin.

[1,2,4,5]Department of Mathematics, Loyola College, Chennai
[3]Panimalar Engineering College, Chennai

Email: [1]jjanetsheeba@loyolacollege.edu, [2]matzpeter@loyolacollege.edu

DOI: 10.31838/ecb/2023.12.s3.726

1. Introduction

One of the first quinolone medications, cinoxacin, was made available in the 1970s. Commonly referred to as quinolones of the first generation. Other quinolone medications from this first generation included pipemidic acid and oxolinic acid, although they only offered slight advantages above nalidixic acid. Oxolinic acid and nalidixic acid share chemical similarities with cipotacin as well as antibacterial properties. It was discovered that cinoxacin had a little higher inhibitory and bactericidal action than nalidixic acid. Eli Lilly received the 1972 patent for cinoxacin [1]. On June 13, 1980, Eli Lilly received FDA approval to market cinoxacin as cinobac in the United States. Previously, in 1979, Switzerland and the United Kingdom began selling cinobac. In accordance with a contract with Eli Lilly, Oclassen Pharmaceuticals (Oclassen Dermatologics) began selling Cinobac in the United States and Canada in September 1992. This deal gave Oclassen exclusive distribution rights in these two countries [2]. Oclassen marketed Cinobac mainly to urologists for the prophylactic and outpatient treatment of acute and chronic urinary tract infections. Prior to being bought by Watson Pharmaceuticals, Inc. in 1997, Oclassen Pharmaceuticals was a privately held pharmaceutical business that was established in 1985. After purchasing Oclassen Pharmaceuticals (Oclassen Dermatologics), also founded in 1985, Watson Pharmaceuticals, Inc. also obtained the marketing rights included in the deal with Eli Lilly to market Cinobac [3]. Cinoxacin is used to prevent and treat infections of the urinary tract. It will not work for other infections or for colds, flu, or other virus infections. Cinoxacin is available only with the doctor's prescription.
Cinoxacin mode of action involves the inhibiting of DNA gyrase, a type II topoisomerase, and topoisomerase iv, which is an enzyme necessary to separate replicated DNA, thereby inhibiting cell division [4]. In this paper, we calculate the topological indices for Cinoxacin, including the Atom-bond connectivity index, Fourth Atom-bond connectivity index, Sum connectivity index, Randic connectivity index, Geometric- arithmetic connectivity index, and Fifth Geometric- arithmetic connectivity index.
The Atom-Bond Connectivity Index, or ABC index, was developed by Estrada et al. [5] in the late 1990s and is one of the degree-based molecular descripters. It can be used to model the thermodynamic properties of organic chemical compounds and to explain the stability of branched alkanes.
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Definition 1. Let $G = (v, E)$ be a molecular graph and d_u is the degree of the vertex u, then *ABC* index of *G* is defined as, $ABC(G) = \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}}$
The fourth atom bond connectivity index, $ABC_4(G)$ index was introduced by M. Ghorbani et al in 2010 [6].

Definition 2. Let *G* be a graph, then its fourth *ABC* index is defined as
$ABC_4\,(G) = \sum_{uv \in E} \sqrt{\frac{S_u + S_v - 2}{S_u\, S_v}}$, where S_u is sum of the degrees of all neighbours of vertex *u* in *G*. In other words, $S_u = \sum_{uv \in E} d_u$, Similarly for S_v.
The first and oldest degree based topological index is Randic index denoted by χ(G) and was introduced by Milan Randi´c in 1975. It provides a quantitative assessment of branching of molecules [7].

Definition 3. For the graph *G* Randic index is defined as, $\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u\, d_v}}$

Definition 4. For a simple connected graph *G*, its Sum connectivity index *S(G)* is defined as, $S(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$.

The Geometric-arithmetic index, *GA(G)* index of a graph *G* was introduced by D. Vukicevic et.al[8].

Definition 5. Let *G* be a graph and $e = uv$ be an edge of *G* then,

$$GA(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The fifth Geometric-arithmetic index, $GA_5(G)$ was introduced by A. Graovac et al [9] in 2011.

Definition 6. For a Graph G, the fifth Geometric-arithmetic index is defined as

$GA_5 = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$, Where S_u is the sum of the degrees of all neighbors of the vertex *u* in *G*, similarly S_v.

A pair of molecular descriptors (or topological index), known as the First Zagreb index $M_1(G)$ and Second Zagreb index $M_2(G)$, first appeared in the topological formula for the total π-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N.Trinajstic[10]. Soon after these indices have been used as branching indices. Later the Zagreb indices found applications in QSPR and QSAR studies. Zagreb indices are included in a number of programs used for the routine computation of topological indices POLLY, DRAGON, CERIUS, TAM, and DISSI. $M_1(G)$ and M(G) were recognize as measures of the branching of the carbonc atom molecular skeleton [11], and since then these are frequently used for structure property modeling. Details on the chemical applications of the two Zagreb indices can be found in the books [12, 13].

Definition 7 For a simple connected graph G, the first and second Zagreb indices were defined as follows $M_1(G) = \sum_{e=uv\in E(G)}(d_u + d_v)$, $M_2(G) = \sum_{e=uv\in E(G)} d_u d_v$
Where d_v denotes the degree (number of first neighbors) of vertex *v* in *G*.
In 2012, M. Ghorbani and N. Azimi [14] defined the Multiple Zagreb topological indices of a graph *G*, based on degree of vertices of *G*.

Definition 8. Let $G = (V, E)$ be a graph and d_u be the degree of a vertex *u*, then augmented Zagreb index is denoted by *AZI(G)* and is defined as *AZI(G)* = $\sum_{uv\in E}\left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$.
The Harmonic index was introduced by Zhong [15]. It has been found that the harmonic index correlates well with the Randic index and with the π-electron energy of benzenoid hydrocarbons.

Definition 9. Let $G = (V, E)$ be a graph and d_u be the degree of a vertex *u* then Harmonic index is defined as $H(G) = \sum_{e=uv\in E(G)} \frac{2}{d_u + d_v}$.
G.H. Shirdel et.al [16] introduced a new distance-based of Zagreb indices of a graph *G* named Hyper-Zagreb Index.
Definition 10. The hyper Zagreb index is defined as, $HM(G) = \sum_{e=uv\in E(G)}(d_u + d_v)^2$

2. Main Results

Theorem 1. The Atom bond connectivity index of cinoxacin is given by, *ABC*($C_{12}H_{10}N_2O_5$) = 14.9347

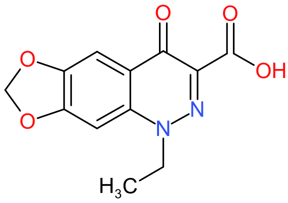

Figure-1

Proof. Consider a cinoxacin $C_{12}H_{10}N_2O_5$. Let $m_{i,j}$ denotes edges connecting the vertices of degrees d_i and d_j. Two dimensional structure if Cinoxacin contains edges of the type $m_{2,2}, m_{2,3}, m_{3,3}, m_{1,2}, m_{1,3}$. From the figure the number of edges of these types are as follows,

$|m_{2,2}| = 2, |m_{2,3}| = 9, |m_{3,3}| = 6, |m_{1,2}| = 1, |m_{1,3}| = 3$

∴ The atom-bond connectivity index of Cinoxacin

$$ABC(G) = \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}}$$

$$= |m_{2,2}|\sqrt{\frac{2+2-2}{2.2}} + |m_{2,3}|\sqrt{\frac{2+3-2}{2.3}} + |m_{3.3}|\sqrt{\frac{3+3-2}{3.3}} + |m_{1.2}|\sqrt{\frac{1+2-2}{1.2}}$$

$$+ |m_{1.3}|\sqrt{\frac{1+3-2}{1.3}}$$

$$=2\left(\sqrt{\frac{1}{2}}\right) + 9\left(\sqrt{\frac{1}{2}}\right) + 6\left(\sqrt{\frac{4}{9}}\right) + 1\left(\sqrt{\frac{1}{2}}\right) + 3\left(\sqrt{\frac{2}{3}}\right) = 14.9347$$

Theorem 2. The fourth atom bond connectivity index of Cinoxacin is

ABC_4($C_{12}H_{10}N_2O_5$) = 11.0257

Proof. Let $e_{i,j}$ denotes the edges of cinoxacin with $i = S_u$ & $j = S_v$. It is easy to see that the summation of degrees of edge endpoints of cinoxacin have the following edge types $e_{4.5}$, $e_{5.7}$, $e_{7.7}$, $e_{6.7}$, $e_{6.8}$, $e_{8.8}$, $e_{7.8}$, $e_{4.7}$, $e_{2.4}$, $e_{3.7}$, $e_{5.8}$ & $e_{3.5}$. From the figure

$|e_{4.5}| = 2$ $|e_{5.7}| = 2$ $|e_{7.7}| = 1$ $|e_{6.7}| = 3$

$|e_{6.8}| = 3$ $|e_{8.8}| = 1$ $|e_{7.8}| = 3$ $|e_{4.7}| = 1$

$|e_{2.4}| = 1$ $|e_{3.7}| = 1$ $|e_{5.8}| = 1$ $|e_{3.5}| = 2$

The fourth atom bond connectivity index of cinoxacin

$$ABC_4\,(G) = \sum_{uv \in E} \sqrt{\frac{S_u + S_v - 2}{S_u\, S_v}}$$

$$= |e_{4.5}|\sqrt{\frac{4+5-2}{4.5}} + |e_{5.7}|\sqrt{\frac{5+7-2}{5.7}} + |e_{7.7}|\sqrt{\frac{7+7-2}{7.7}} + |e_{6.7}|\sqrt{\frac{6+7-2}{6.7}}$$

$$+ |e_{6.8}|\sqrt{\frac{6+8-2}{6.8}} + |e_{8.8}|\sqrt{\frac{8+8-2}{8.8}} + |e_{7.8}|\sqrt{\frac{7+8-2}{7.8}} + |e_{4.7}|\sqrt{\frac{4+7-2}{4.7}}$$

$$+ |e_{2.4}|\sqrt{\frac{2+4-2}{2.4}} + |e_{3.7}|\sqrt{\frac{3+7-2}{3.7}} + |e_{5.8}|\sqrt{\frac{5+8-2}{5.8}} + |e_{3.5}|\sqrt{\frac{3+5-2}{3.5}}$$

$= 2\sqrt{\frac{7}{20}} + 2\sqrt{\frac{10}{35}} + 1\sqrt{\frac{12}{49}} + 3\sqrt{\frac{11}{42}} + 3\sqrt{\frac{12}{48}} + 1\sqrt{\frac{14}{64}} + 3\sqrt{\frac{13}{56}}$

$+1\sqrt{\frac{9}{28}} + 1\sqrt{\frac{4}{8}} + 1\sqrt{\frac{8}{21}} + 1\sqrt{\frac{11}{40}} + 2\sqrt{\frac{6}{15}}$

$= 11.0257$

Theorem 3. The Randic connectivity index of cinoxacin □ ($C_{12}H_{10}N_2O_5$) = 9.1133

Proof. Consider Randic connectivity index of Cinoxacin $\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u\, d_v}}$

$= |m_{2.2}| \frac{1}{\sqrt{(2.2)}} + |m_{2.3}| \frac{1}{\sqrt{(2.3)}} + |m_{3.3}| \frac{1}{\sqrt{(3.3)}} + |m_{1.2}| \frac{1}{\sqrt{(1.2)}} + |m_{1.3}| \frac{1}{\sqrt{(1.3)}}$

$= 2\frac{1}{\sqrt{(4)}} + 9\frac{1}{\sqrt{(6)}} + 6\frac{1}{\sqrt{(3)}} + 1\frac{1}{\sqrt{(2)}} + 3\frac{1}{\sqrt{(3)}}$

$= 9.1133$

Theorem 4. The sum of connectivity index of Cinoxacin $S(C_{12}H_{10}N_2O_5) = 9.5517$

Proof. Consider the sum connectivity index of Cinoxacin $S(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$.

$= |m_{2.2}| \frac{1}{\sqrt{(2+2)}} + |m_{2.3}| \frac{1}{\sqrt{(2+3)}} + |m_{3.3}| \frac{1}{\sqrt{(3+3)}} + |m_{1.2}| \frac{1}{\sqrt{(1+2)}} + |m_{1.3}| \frac{1}{\sqrt{(1+3)}}$

$= 2\frac{1}{\sqrt{(4)}} + 9\frac{1}{\sqrt{(5)}} + 6\frac{1}{\sqrt{(6)}}\ 1\frac{1}{\sqrt{(3)}} + 3\frac{1}{\sqrt{(4)}} = 9.5517$

Theorem 5. The Geometric-Arithmetic index of Cinoxacin

$GA(G) = \sum_{e= uv\in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u + d_v} = 18.6269$

Proof. Consider the Geometric-Arithmetic index of Cinoxacin

$GA(G) = \sum_{e= uv\in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u + d_v}$

$= 2\, [\ |m_{2,2}| \frac{\sqrt{2.2}}{2+2} + |m_{2,3}| \frac{\sqrt{2.3}}{2+3} + |m_{3,3}| \frac{\sqrt{3.3}}{3+3} + |m_{1,2}| \frac{\sqrt{1.2}}{1+2} + |m_{1,3}| \frac{\sqrt{1.3}}{1+3}\ ]$

$= 2\, [\ 2\frac{\sqrt{4}}{4} + 9\frac{\sqrt{6}}{5} + 6\ \frac{\sqrt{9}}{6} + 1\frac{\sqrt{2}}{3} + 1.\ \frac{\sqrt{3}}{4}\ ]$

$= 18.6269$

Theorem 6. The fifth Geometric-Arithemetic index of Cinoxacin $GA_5 = \sum_{uv\in E(G)} \frac{2\sqrt{S_u\ S_v}}{S_u + S_v}$

$GA_5(C_{12}H_{10}N_2O_5) = 20.64422$

Proof. Consider the fifth Geometric-Arithemetic index of Cinoxacin

$$GA_5 = \sum_{uv\in E(G)} \frac{2\sqrt{S_u\ S_v}}{S_u + S_v}$$

$= 2\, [\, |e_{6.7}| \sqrt{\frac{6.7}{6+7}} + |e_{4.5}| \sqrt{\frac{4.5}{4+5}} + |e_{5.7}| \sqrt{\frac{5.7}{5+7}} + |e_{7.7}| \sqrt{\frac{7.7}{7+7}}$

$+ |e_{6.8}| \sqrt{\frac{6.8}{6+8}} + |e_{8.8}| \sqrt{\frac{8.8}{8+8}} + |e_{7.8}| \sqrt{\frac{7.8}{7+8}} + |e_{4.7}| \sqrt{\frac{4.7}{4+7}}$

$+ |e_{2.4}| \sqrt{\frac{2.4}{2+4}} + |e_{3.7}| \sqrt{\frac{3.7}{3+7}} + |e_{5.8}| \sqrt{\frac{5.8}{5+8}} + |e_{3.5}| \sqrt{\frac{3.5}{3+5}}\,]$

$= 2\, [\ 2\frac{\sqrt{20}}{9} + 2\ \frac{\sqrt{35}}{12} + \frac{\sqrt{49}}{14} + 3\frac{\sqrt{42}}{13} + 3\ \frac{\sqrt{48}}{14} + \frac{8}{16} + 3\frac{\sqrt{56}}{15} + \frac{\sqrt{28}}{11} + \frac{\sqrt{8}}{6} + \frac{\sqrt{21}}{10} + \frac{\sqrt{40}}{13} + 2\frac{\sqrt{15}}{8}$

= 20.64422

Theorem 7(a). The First Zagreb index of Cinoxacin is $M_1(C_{12}H_{10}N_2O_5)$ = 113
Proof. Consider First Zagreb index of Cinoxacin is $M_1(G) = \sum_{e=uv \in E(G)}(d_u + d_v)$
= $|m_{2,2}|(2+2) + |m_{2,3}|(2+3) + |m_{3,3}|(3+3) + |m_{1,2}|(1+2) + |m_{1,3}|(1+3)$
= 2(4) + 9(6) + 6(6) + 1(3) + 3(4)
= 8 + 54 + 36 + 3 + 12
= 113

Theorem 7(b). The Second Zagreb index of Cinoxacin is $M_2(C_{12}H_{10}N_2O_5)$ = 127
Proof. The Second Zagreb index of Cinoxacin is $M_2(G) = \sum_{e=uv \in E(G)} d_u d_v$
$M_2(G) = |m_{2,2}|(2.2) + |m_{2,3}|(2.3) + |m_{3,3}|(3.3) + |m_{1,2}|(1.2) + |m_{1,3}|(1.3)$
= 2(4) + 9(6) + 6(9) + 1(2) + 3(3)
= 8 + 54 + 54 + 2 + 9 = 127

Theorem 8. The Augmented Zagreb index of Cinoxacin $AZI(G) = \sum_{uv\in E}\left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$
$AZI(C_{12}H_{10}N_2O_5)$ = 174.46875
Proof. The augmented Zagreb index of Cinoxacin is $AZI(G) = \sum_{uv\in E}\left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$
$AZI(G) = |m_{2,2}|\left[\frac{2.2}{2+2-2}\right]^3 + |m_{2,3}|\left[\frac{2.3}{2+3-2}\right]^3 + |m_{3,3}|\left[\frac{3.3}{3+3-2}\right]^3 + |m_{1,2}|\left[\frac{1.2}{1+2-2}\right]^3$
$+ |m_{1,3}|\left[\frac{1.3}{1+3-2}\right]^3$
$=2(2)^3 + 9(2)^3 + 6\left(\frac{9}{4}\right)^3 + 1(2)^3 + 3\left(\frac{3}{2}\right)^3$
= 174.46875

Theorem 9. The harmonic index of Cinoxacin is $H(G) = \sum_{e=uv \in E(G)} \frac{2}{d_u + d_v}$
$H(C_{12}H_{10}N_2O_5)$ = 8.76666
Proof. The harmonic index of Cinoxacin is $H(G) = \sum_{e=uv \in E(G)} \frac{2}{d_u + d_v}$
$= 2\ [\ |m_{2,2}|\left[\frac{1}{2+2}\right] + |m_{2,3}|\left[\frac{1}{2+3}\right] + |m_{3,3}|\left[\frac{1}{3+3}\right] + |m_{1,2}|\left[\frac{1}{1+2}\right] + |m_{1,3}|\left[\frac{1}{1+3}\right]$
$= 2\ [\ 2\left(\frac{1}{4}\right) + 9\left(\frac{1}{5}\right) + 6\left(\frac{1}{6}\right) + 1\left(\frac{1}{3}\right) + 3\left(\frac{1}{4}\right)$
=8.76666

Theorem 10. The hyper Zagreb index of Cinoxacin is $HM(G) = \sum_{e=uv \in E(G)}(d_u + d_v)^2$
$HM(C_{12}H_{10}N_2O_5)$ =230
Proof. The hyper Zagreb index of Cinoxacin is $HM(G) = \sum_{e=uv \in E(G)}(d_u + d_v)^2$
$= |m_{2,2}|(2+2)^2 + |m_{2,3}|(2+3)^2 + |m_{3,3}|(3+3)^2 + |m_{1,2}|(1+2)^2 + m_{1,3}|(1+3)^2$
= 2(16) + 9(25) + 6(36) + 1(9) + 3(16)
= 32 + 216 + 225 + 9 + 48
= 530

3. Conclusion

ABC index, ABC_4 index, Randic connectivity index, sum connectivity index, GA index, GA_5 index, first Zagreb index, second Zagreb index, augmented Zagreb index, Harmonic index and hyper Zagreb index of Cinoxacin were calculated.

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