Degree-Based and Degree-Splitting Topological Indices of Salbutamol

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ABSTRACT

The drug Salbutamol aids in the lungs medium and broad airway enlargement. Treatment for acute episodes of bronchospasm caused by bronchial asthma, chronic bronchitis, and other long-term bronchopulmonary disorders including chronic obstructive pulmonary disease (COPD) usually involves its use. In this work, the degree-based and degree splitting topological indices of salbutamol are computed using both a Python software and manual calculation. Furthermore, QSAR analysis of the topological indices are discussed using SPSS

Keywords: Salbutamol, Topological indices, Degree Splitting graphs, Python Programming, SPSS

Subject Classification: 05C07, 05C09, 05C92

1. INTRODUCTION

A topological index of graph G is a numerical value that describes its topology. It reflects the theoretical characteristics of a chemical molecule when applied to its molecular structure. In this study, chemical structures of drugs used to treat asthma were subjected to well-known degree-based topological indices. Chemical structure is viewed as a graph, where the constituents are the vertices and the boundaries between them are the edges.

Salbutamol is a member of the group of drugs known as bronchodilators, more specifically, 2-adrenergic agonists. This medicine is used to treat and prevent bronchospasm caused by respiratory illnesses like chronic bronchitis, asthma, and other breathing problems.

2. PRELIMINARIES

In this section, certain well-known definitions and findings concerning various topological indices of graphs are described for quick reference while one reads the material presented in this paper.

Definition 2.1: The degree of a vertex v in G or simply d(v) is the number of edges of G incident with vertex v.

Definition 2.2: ABC (atom bond connectivity) index of a graph G defined in [2] as, ABC(G) (atom bond connectivity) index of a graph G in as,

$$\mathrm{ABC(G)} = \sum_{pq\epsilon\, E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

Definition 2.3: ABS (atom bond sum connectivity) index of a graph G defined in [1] as $\mathrm{ABS(G)} = \sum_{pq\epsilon\, E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$

Definition 2.4: ABS (atom bond sum connectivity) index of a graph G defined in [1] as $\mathrm{AZI(G)} = \sum_{pq\epsilon\, E(G)} \left(\sqrt{\frac{d(u)d(v)}{d(u)+d(v)-2}}\right)^3$

Definition 2.5:SAI (sum augmented index) is defined in [4] as,

$$\mathrm{SAI(G)} = \sum_{pq\epsilon\, E(G)} \left(\sqrt{\frac{d(u) + d(v)}{d(u) + d(v) - 2}}\right)^3$$

Definition 2.6: GA (geometric-arithmetic index)of a graph G is defined in [8] as

$$\mathrm{GA(G)} = \sum_{pq\epsilon\, E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

Definition 2.7:AG (Arithmetic-geometric index) of a graph G is defined in [8] as

$$\mathrm{AG(G)} = \sum_{pq\epsilon\, E(G)} \frac{d(u) + d(v)}{2\sqrt{d(u)d(v)}}$$

Definition 2.8:GO1(first Gourava index) and GO2 (second Gourava index) of a graph G are defined in [5] as,

$$GO1(G) = \sum_{pq\epsilon\, E(G)} \left[\left(d(u) + d(v)\right) + d(u)d(v)\right]$$

$$GO2(G) = \sum_{pq\epsilon\, E(G)} \left[\left(d(u) + d(v)\right) d(u)d(v)\right]$$

Definition 2.9: HGO1(first hyper Gourava index) and HGO2 (second hyper Gouravaindex)of a graph G are defined in [6] as,

$$HGO1(G) = \sum_{pq\epsilon\, E(G)} (d(u) + d(v) + d(u)d(v))^2$$

$$HGO2(G) = \sum_{pq\epsilon\, E(G)} (d(u) + d\,(v)d(u)d(v))^2.$$

Definition 2.10 : Let G= (V,E) be a graph with V= S_1US_2…..UT where each Si is a set of vertices having at least two vertices , having the same degree and T = V\ USi. The Degree splitting of Graph denoted by DS(G) is obtained from G by adding new vertices w_1, w_2..w_i and joining w_i to each vertex of S_i

3. Topological Indices of Salbutamol

The several topological indices of salbutamol are covered in this section. Salbutamol has 17 vertices and 17 edges in its chemical graph. The graph below displays salbutamol's chemical structure.

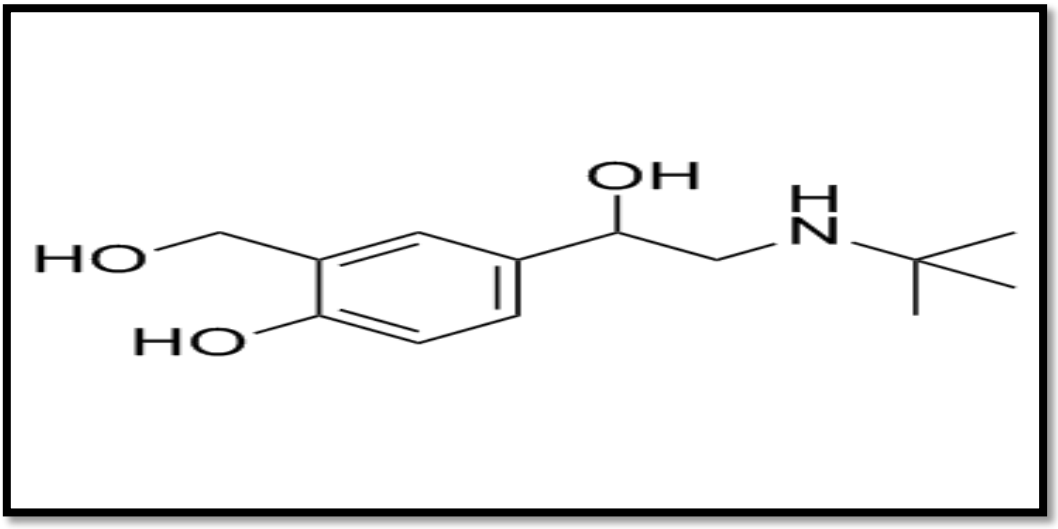

Figure 1 : Chemical Structure of Salbutamol

Table 1. Edge partition of Salbutamol

(d(u),d(v))/(u,v) ∈E(G)	Number of edges
(1,2)	1
(1,3)	2
(1,4)	3

(2,2)	2
(2,3)	6
(2,4)	1
(3,3)	2

Theorem 1: ABC index of Salbutamol is ABC(G) = 12.6348

Proof: From definition 2.2

$$\mathrm{ABC(G)} = \sum_{pq\epsilon\, E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

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

= 12.6348

By using Python Programming, the ABC of Salbutamol is also calculated.

```
#ABC(G)
import math
for i in range(1,8):
  a=int(input("enter a value:"))
  b=int(input("enter b value:"))

  if a==1 and b==2:
    c=(a+b-2)/(a*b)
    print(c)
    c1_ans=math.sqrt(c)
    mul1=c1_ans*1
    print(mul1)


  if a==1 and b==3:
     c=(a+b-2)/(a*b)
     print(c)
     c2_ans=math.sqrt(c)
     mul2=c2_ans*2
     print(mul2)

  if a==1 and b==4:
     c=(a+b-2)/(a*b)
     print(c)
     c3_ans=math.sqrt(c)
     mul3=c3_ans*3
```

```
    print(mul3)


  if a==2 and b==2:
    c=(a+b-2)/(a*b)
    print(c)
    c4_ans=math.sqrt(c)
    mul4=c4_ans*2
    print(mul4)
  if a==2 and b==3:
    c=(a+b-2)/(a*b)
    print(c)
    c5_ans=math.sqrt(c)
    mul5=c5_ans*6
    print(mul5)

  if a==2 and b==4:
    c=(a+b-2)/(a*b)
    print(c)
    c6_ans=math.sqrt(c)
    mul6=c6_ans*1
    print(mul6)

  if a==3 and b==3:
    c=(a+b-2)/(a*b)
    print(c)
    c7_ans=math.sqrt(c)
    mul7=c7_ans*2
    print(mul7)

final=mul1+mul2+mul3+mul4+mul5+mul6+mul7
print(final)
```

Output of the above program

```
enter a value:1
enter b value:2
0.5
0.7071067811865476

enter a value:1
enter b value:3
0.6666666666666666
1.632993161855452

enter a value:1
enter b value:4
0.75
2.598076211353316

enter a value:2
enter b value:2
0.5
```

```
1.4142135623730951

enter a value:2
enter b value:3
0.5
4.242640687119286

enter a value:2
enter b value:4
0.5
0.7071067811865476

enter a value:3
enter b value:3
0.4444444444444444
1.3333333333333333
```

12.635470518407578

Similarly, the other topological indices from Definition 2.3 to 2.9 are calculated by both analytically and using Python programming which are listed in the table below:

Topological Index	Topological Index of Salbutamol
ABC	12.6354
ABS	12.8266
AZI	116.6424
SAI	110.7916
GA	15.782
AG	18.3044
GO1	250
GO2	458
HGO1	7248
HGO2	15572

4. Topological Indices of Degree Splitting of Salbutamol

The different topological indices of Salbutamol's degree splitting are assessed in this section. The degree splitting graph of salbutamol consists of 21 vertices and 34 edges.

Table 2. Edge Partition of degree Splitting of Salmabutamol

(d(u),d(v))/(u,v)∈(G)	Number of edges
(1,5)	1
(2,3)	2
(2,4)	2
(2,5)	3
(2,6)	6
(3,3)	2
(3,4)	5
(3,5)	1
(3,6)	6
(4,4)	6

The topological indices from Definition 2.2 to 2.9 are calculated by both analytically and using Python programming which are listed in the table below:

Topological Index	Degree Splitting Topological Index of Salbutamol
ABC	22.6959
ABS	28.9427
AZI	433.2746
SAI	91.6532
GA	30.8491
AG	36.2013
GO1	1011
GO2	3360
HGO1	48111
HGO2	388584

5. Comparison Between Salbutamol & Degree Splitting Graph of Salbutamol

This section presents the correlation coefficient, as determined by a regression model, between Salbutamol's topological indices and its degree splitting graph. Using the SPSS software and the data in Tables 1 and 2, the linear and quadratic models are produced.

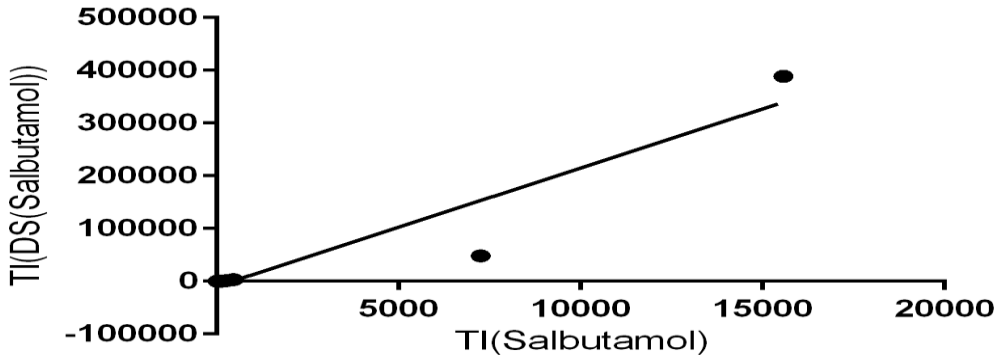

Figure 1

Best-fit values

Slope	22.42 ± 2.696
Y-intercept	-9224 ± 14649
X-intercept	411.4
1/Slope	0.04460

95% Confidence Intervals

Slope	16.20 to 28.64
Y-intercept	-43005 to 24558
X-intercept	-1281 to 1776

Goodness of Fit

R square	0.8963
Sy.x	41640

Is slope significantly non-zero?

F	69.18
DFn,DFd	1,8
P Value	< 0.0001
Deviation from horizontal?	Significant

Data

Number of XY pairs	10
Equation	Y = 22.42*X - 9224

6.Conclusion

Salbutamol's degree based topological indices and degree splitting topological indices are examined using degree-based indices. A graphical comparison of the computed findings for the chemical compounds stated above may be found in Figure 1. The creation of novel drugs to treat chronic bronchitis, bronchial asthma, and other long-term bronchopulmonary conditions may benefit from these discoveries.

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