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Neighbourhood Sum VDB Indices and Entropy for Specific Types of Molecular Graphs

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Abstract:

Introduction: Numerous TIs for different molecular graphs have been found and studied. The entropy measurements and the neighbourhood sum degree-based M-polynomial are derived for the six different anti-asthmatic drugs by using a set of 19 degree-based topological indices in this article.

Objectives: Develop the neighbourhood sum degree-based M-polynomial for different anti-asthmatic drugs to characterize their molecular graphs. Compare the entropy measurements obtained for them.

Methods: Based on these molecular descriptors, it is practical and effective to analyse the mathematical values and conduct additional research on a molecule's numerous physical properties. They offer helpful substitutes for drawn-out, costly, and labour-intensive laboratory investigations. Using quantitative structure-activity relationships (QSARs) and quantitative structure-property relationships (QSPRs), the topological indices can be utilized to predict chemical structures, physicochemical properties, and biological activities.

Results: Based on their matching molecular structures, the topological indices of the six different anti-asthmatic drugs are determined in this article.

Conclusions: A graphical comparison of the calculated indices is made to examine how they relate to the molecular structure and to one another.

Keywords: Degree-based indices, M-Polynomial, entropy measures, and neighborhood sum degree-based indices.

1. Introduction

The primary techniques for theoretically investigating chemical compounds are increasingly graph theoretical tools. These methods are crucial to the creation of new, more effective herbicides since their properties can be estimated prior to synthesis. Furthermore, QSPR/QSAR models can replace experimental measurements because they are less ex pensive and time-consuming.

In this context, topological indices provide a numerical representation of molecular topology. The computation of TIs can be done effectively and practically using algebraic polynomials. With this method, estimating several TIs is reduced to computing a single polynomial. For example, to find TIs based on distance, the Hosoya polynomial is widely employed. Deutsch and Klavˇzar created a comparable polynomial for the degree-based index calculation. By using this technique

, several important degree-based benchmarks are computed using a single polynomial, known as the M-polynomial. Numerous scholarly works address the M-polynomial and its application in the computation of degree-based indices. The degree-based entropy measures are computed for these structures. The neighbourhood sum degree-based TIs are one recent development in the application of graph theory to chemical compound research. The degree-based entropy metrics that are widely studied and employed in graph theory are considered information functionals in the study of networks. Applications of entropy network measures include the study of the chemical and biological properties of molecular graphs and the quantitative description of a molecule's structure. We consider a simple connected graph that has few edges and no self-loops.

The graph $\mathfrak{G}$ is referred to as a connected graph when $V(\mathfrak{G})$ and $E(\mathfrak{G})$ represent the vertex set and edge set, respectively. The degree of the vertex is indicated by the symbol $d\mathfrak{v}$.

The neighbourhood sum degree-based TI's are denoted by $\mathfrak{N}_{\mathfrak{G}}(\mathfrak{v})$. The neighbourhood sum degree of the molecular graph is written as $|\boldsymbol{\mathfrak{N}_{\mathfrak{G}}(\mathfrak{v})}| = \boldsymbol{d\mathfrak{v}}$. The $\boldsymbol{\mathfrak{N}_{\mathfrak{G}}(\mathfrak{v})}$ denotes the sum of the degrees of vertices that are next to $\boldsymbol{\mathfrak{v}}$. Let's start by building the M-polynomial of $\boldsymbol{\mathfrak{G}}$ based on the neighbourhood sum degree:

$$\mathfrak{N}\mathfrak{M}(\mathfrak{G}) = \Sigma_{(i\leq j)}(\text{Number of all edges } \mathfrak{u}\mathfrak{v} \text{ such that } \mathrm{H}\mathfrak{u} = \mathrm{i}, \mathrm{H}\mathfrak{v} = \mathrm{j})l^i p^j$$

$$\mathfrak{D}(\mathfrak{G}) = \Sigma_{\mathfrak{u}\mathfrak{v}\in\mathbb{E}(\mathfrak{G})} g(\varphi_u \varphi_v) \; and \; \mathfrak{N}\mathfrak{M}(\mathfrak{G}) = \Sigma_{\mathfrak{u}\mathfrak{v}\in\mathbb{E}(\mathfrak{G})} g(\mathfrak{w}_u \mathfrak{w}_v)$$

1	$M_1(\mathfrak{G}) = D_n + D_v(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	First Zagreb Index
2	$M_2(\mathfrak{G}) = D_n * D_v(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	Second Zagreb Index
3	$M_2^m(\mathfrak{G}) = S_n * S_v(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	Second modified Zagreb Index
4	$D_n^\alpha * D_v^\alpha(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	General Randic Index
5	$S_n^\alpha * S_v^\alpha(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	Inverse Randic Index
6	$[D_n S_v + D_n S_v](\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	Symmetric Division Index
7	$2S_n J(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=1)}$	Harmonic Index
8	$S_n J D_n D_v(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=1)}$	Inverse Sum Index
9	$\mathbb{S}_s^3 Q_{-2} J\mathbb{D}_s^3 \mathbb{D}_p^3(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=1)}$	Augumented Redefined Zagreb Index
10	$[D_n + D_v][S_n.S_v]^{-1}(\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	First Redefined Zagreb Index
11	$[D_n * D_v][D_n + D_v](\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=h=1)}$	Third Redefined Zagreb Index
12	$D_n^{1/2} Q_{-2} J[S_n^{1/2}.S_n^{1/2}](\mathfrak{N}\mathfrak{M}(\mathfrak{G}: g, h))\vert_{(g=1)}$	Atom–bond sum Index

13	$D_n^{1/2} Q_{-2} J[S_n^{1/2} + S_n^{1/2}](\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=1)}$	Atom–bond Connectivity Index
14	$[D_n^2 + D_n^2](\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=h=1)}$	F-Index
15	$\frac{1}{4}[D_g + D_h]^2(\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=h=1)}$	Second Shigehalli and Kanaburs Index
16	$[D_n^{1/2} * D_n^{1/2}](\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=h=1)}$	Reciprocal Randic Index
17	$[D_g + D_h]^{-1}(\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=h=1)}$	General Sum-connectivity Index
18	$\frac{1}{2}[D_n * D_v][D_n + D_v]^{(-\frac{1}{2})}(\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=h=1)}$	Arithmetic Geometric Index
19	$2[D_n D_v]^{\frac{1}{2}}[D_n + D_v]^{(-1)}(\mathfrak{NM}(\mathfrak{G}: g, h))\|_{(g=h=1)}$	Geometric Arithmetic Index

Table1abovelists theNM-Polynomialderivatives[11,10,17,1]

2. Neighbourhood Degree Sum-Based Entropy Measures:

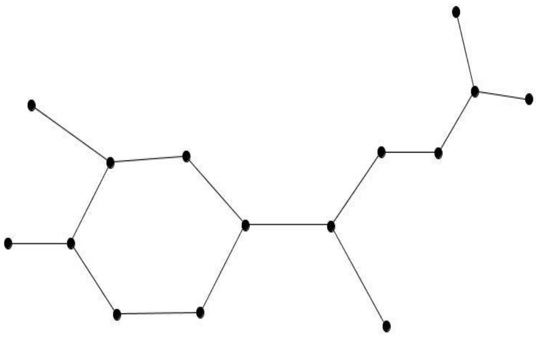
In his seminal work, Shannon defined entropy as a means of quantifying the degree of uncertainty in a system or the unexpectedness of relevant information. The structural informativeness of a network has been measured using entropy computations [18]. Information theory has been widely applied because of its versatility in many different domains, including linguistics, electrical engineering, chemical and medical sciences, and graph theory for chemical networks[6,5]. A method for measuring the topological information of chemical networks and graphs was introduced graph entropy.

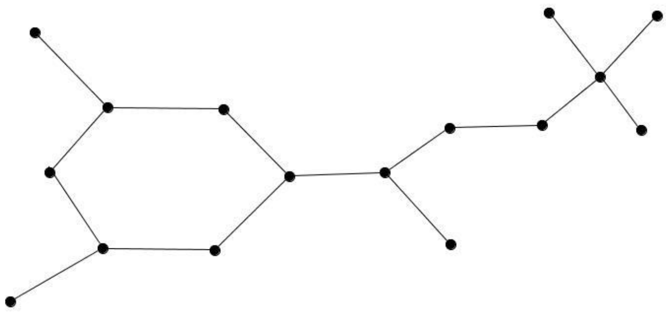
[19, 16] Rashevsky computed graph entropy using vertex orbits. Using intrinsic and extrinsic graph entropy measurements, mathematicians may relate probability distributions to graph elements such as vertices and edges. Graph entropies are widely used in many fields, including as biology, ecology, chemistry, and sociology. [5, 7] Dehmer created graph entropies and used information functional analysis to extract structural information from them. $ENT_{\mathfrak{G}} = \Sigma_{j=1}^{b_i} p_{ij} logp$. If $\mathfrak{G} = (V, E, w)$ is an edge-weighted graph then the entropy measure of G is defined as [4, 8].

$$\mathbf{ENT_{\mathfrak{G}}} = \boldsymbol{log_{\Omega}(\mathfrak{G})} - \frac{\mathbf{1}}{\boldsymbol{\Omega(\mathfrak{G})}} \boldsymbol{\Sigma_{\mathfrak{uv}\in\mathbb{E}(\mathfrak{G})} F(\mathfrak{d}_u \mathfrak{d}_v) log(F(\mathfrak{d}_u \mathfrak{d}_v))}$$

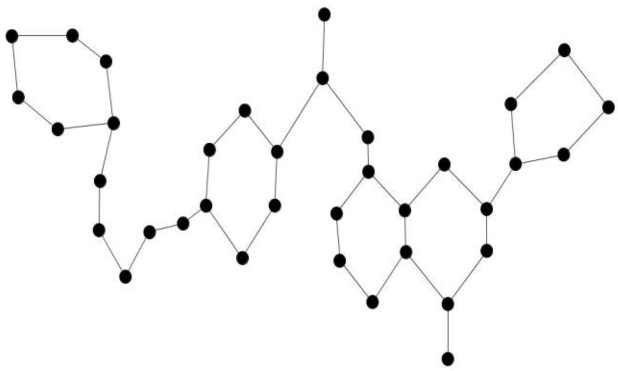
3.Computing Neighbourhood Sum Degree-Based M - polynomial by Using TI's.

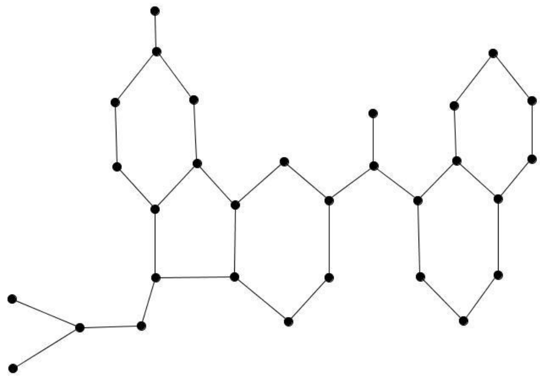
We compute the NM-Polynomials for isoproterenol, terbutaline, pranlukast, setipiprant, bedoradrine and toreforant. These drugs are often used as part of a comprehensive treatment plan for asthma and COPD, either alone or in combination with other medications such as inhaled corticosteroids or short-acting beta agonists. It's important to use them as prescribed by a healthcare professional and to be aware of their potential side effects and interactions. The below graphs are indicating their molecular graphs.



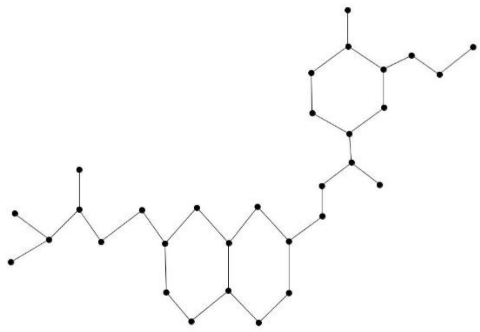


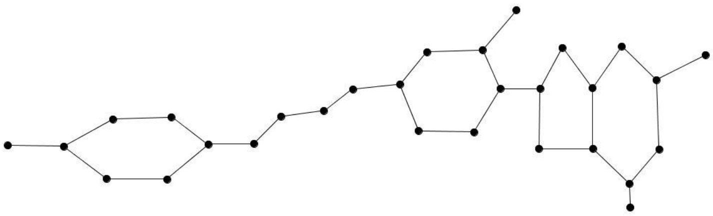
a) Isoproterenol b) Terbutaline





c) Pranlukast d) Setipiprant





e) Bedoradrine f) Toreforant

Figure.1. Anti-Asthmatic-Drugs

(d_u, d_v)	Frequency
(3,4)	2
(3,6)	3
(4,5)	1
(5,5)	2
(5,6)	2
(5,7)	1
(6,6)	2
(6,7)	2

(d_u, d_v)	Frequency
(3,5)	2
(3,6)	1
(4,5)	3
(5,6)	7
(6,7)	3

Table 3: Partition table for terbutaline

Table 2: Partition table for isoproterenol

(d_u, d_v)	Frequency
3,6)	2
(4,4)	5
(4,5)	8
(5,5)	2
(5,6)	6
(5,7)	5

(d_u, d_v)	Frequency
(3,4)	1
(3,5)	2
(3,7)	1
(4,5)	5
(4,6)	1
(5,5)	3
(5,6)	1
(5,7)	3
(5,8)	4
(6,7)	1
(6,8)	3
(7,7)	1
(7,8)	2
(8,8)	6

(5,8)	1
(6,6)	2
(6,7)	4
(6,8)	2
(7,7)	1
(7,8)	1
(8,8)	1

Table 4: Partition table for pranlukast   Table 5: Partition table for setipiprant

$(\mathfrak{d}_{\mathfrak{u}}, \mathfrak{d}_{\mathfrak{v}})$	**Frequency**
(2,3)	1
(3,5)	3
(3,6)	3
(5,5)	5
(5,6)	8
(5,7)	4
(6,6)	2
(6,7)	6
(7,7)	1

$(\mathfrak{d}_{\mathfrak{u}}, \mathfrak{d}_{\mathfrak{v}})$	**Frequency**
(3,5)	2
(3,6)	2
(4,4)	1
(4,5)	2
(5,5)	5
(5,6)	7
(5,8)	1
(6,6)	3
(6,7)	4
(6,8)	5

Table 6: Partition table for bedoradrine

Table 7: Partition table for toreforant

Theorem 3.1. Given that $\mathfrak{G}$ to be a isoproterenol, the following $\mathfrak{NM}$ -polynomial of $\mathfrak{G}$. $\mathfrak{NM}(\mathfrak{G}, g, h) = 2g^3h^4 + 3g^3h^6 + g^4h^5 + 2g^5h^5 + 2g^5h^6 + g^5h^7 + 2g^6h^6 + 2g^6h^7$

Theorem 3.2. If $\mathfrak{G}$ is a isoproterenol, then that $\mathfrak{G}$′s NM -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 154$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 399$
3. $\mathfrak{NM}_{M_2^m}(\mathfrak{G}) = 0.66175$

4. $\mathfrak{NM}_{GRI}(\mathfrak{G}) = 399$
5. $\mathfrak{NM}_{IRI}(\mathfrak{G}) = 0.66175$
6. $\mathfrak{NM}_{SDI}(\mathfrak{G}) = 31.945$
7. $\mathfrak{NM}_{HI}(\mathfrak{G}) = 3.0316$
8. $\mathfrak{NM}_{ISI}(\mathfrak{G}) = 37.484$
9. $\mathfrak{NM}_{AZ}(\mathfrak{G}) = 484.6$
10. $\mathfrak{NM}_{ReZ_1}(\mathfrak{G}) = 6.2786$
11. $\mathfrak{NM}_{ReZ_3}(\mathfrak{G}) = 4370$
12. $\mathfrak{NM}_{ABC}(\mathfrak{G}) = 8.5924$
13. $\mathfrak{NM}_{ABS}(\mathfrak{G}) = 13.394$
14. $\mathfrak{NM}_{F}(\mathfrak{G}) = 836$
15. $\mathfrak{NM}_{SK_2}(\mathfrak{G}) = 408.5$
16. $\mathfrak{NM}_{RR}(\mathfrak{G}) = 75.959$
17. $\mathfrak{NM}_{SI}(\mathfrak{G}) = 4.7455$
18. $\mathfrak{NM}_{GA_1}(\mathfrak{G}) = 15.237$
19. $\mathfrak{NM}_{AG}(\mathfrak{G}) = 14.774$

Theorem 3.3. Given that $\mathfrak{G}$ to be a terbutaline, the following $\mathfrak{NM}$ -polynomial of $\mathfrak{G}$.
$\mathfrak{NM}(\mathfrak{G}, g, h) = 2g^3h^5 + g^3h^6 + 3g^4h^5 + 7g^5h^6 + 3g^6h^7$

Theorem 3.4. If $\mathfrak{G}$ is a terbutaline, then that $\mathfrak{G}$'s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 168$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 444$
3. $\mathfrak{NM}_{M_2^m}(\mathfrak{G}) = 0.64365$
4. $\mathfrak{NM}_{GRI}(\mathfrak{G})^2 = 444$
5. $\mathfrak{NM}_{IRI}(\mathfrak{G}) = 0.64365$
6. $\mathfrak{NM}_{SDI}(\mathfrak{G}) = 33.488$
7. $\mathfrak{NM}_{HI}(\mathfrak{G}) = 3.1232$
8. $\mathfrak{NM}_{ISI}(\mathfrak{G}) = 41.2$
9. $\mathfrak{NM}_{AZ}(\mathfrak{G}) = 544.47$
10. $\mathfrak{NM}_{ReZ_1}(\mathfrak{G}) = 6.4119$
11. $\mathfrak{NM}_{ReZ_3}(\mathfrak{G}) = 4890$
12. $\mathfrak{NM}_{ABC}(\mathfrak{G}) = 9.0236$

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13. $\mathfrak{NM}_{ABS}(\mathfrak{G}) = 14.35$
14. $\mathfrak{NM}_{F}(\mathfrak{G}) = 918$
15. $\mathfrak{NM}_{SK_2}(\mathfrak{G}) = 451.5$
16. $\mathfrak{NM}_{RR}(\mathfrak{G}) = 83.188$
17. $\mathfrak{NM}_{SI}(\mathfrak{G}) = 4.9831$
18. $\mathfrak{NM}_{GA_1}(\mathfrak{G}) = 16.183$
19. $\mathfrak{NM}_{AG}(\mathfrak{G}) = 15.823$

Theorem 3.5. Given that $\mathfrak{G}$ to be a pranlukast, the following $\mathfrak{NM}$ -polynomial of $\mathfrak{G}$.
$\mathfrak{NM}(\mathfrak{G}; g, h) = 2g^3h^6 + 5g^4h^4 + 8g^4h^5 + 2g^5h^5 + 6g^5h^6 + 5g^5h^7 + g^5h^8 + 2g^6h^6 + 4g^6h^7 + 2g^6h^8 + g^7h^7 + g^7h^8 + g^8h^8$

Theorem 3.6. If $\mathfrak{G}$ is a pranlukast, then that $\mathfrak{G}$'s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 438$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 1226$
3. $\mathfrak{NM}_{M_2^m}(\mathfrak{G}) = 1.5178$
4. $\mathfrak{NM}_{GRI}(\mathfrak{G}) = 1226$
5. $\mathfrak{NM}_{IRI}(\mathfrak{G}) = 1.5178$
6. $\mathfrak{NM}_{SDI}(\mathfrak{G}) = 82.676$
7. $\mathfrak{NM}_{HI}(\mathfrak{G}) = 7.3359$
8. $\mathfrak{NM}_{ISI}(\mathfrak{G}) = 107.82$
9. $\mathfrak{NM}_{AZ}(\mathfrak{G}) = 1548.6$
10. $\mathfrak{NM}_{ReZ_1}(\mathfrak{G}) = 15.431$
11. $\mathfrak{NM}_{ReZ_3}(\mathfrak{G}) = 14446$
12. $\mathfrak{NM}_{ABC}(\mathfrak{G}) = 22.201$

13. $\mathfrak{NM}_{\mathrm{ABS}}(\mathfrak{G}) = 35.818$
14. $\mathfrak{NM}_{\mathrm{F}}(\mathfrak{G}) = 2526$
15. $\mathfrak{NM}_{\mathrm{SK}_2}(\mathfrak{G}) = 1244.5$
16. $\mathfrak{NM}_{\mathrm{RR}}(\mathfrak{G}) = 217.28$
17. $\mathfrak{NM}_{\mathrm{SI}}(\mathfrak{G}) = 12.203$
18. $\mathfrak{NM}_{\mathrm{GA}_1}(\mathfrak{G}) = 40.33$
19. $\mathfrak{NM}_{\mathrm{AG}}(\mathfrak{G}) = 39.681$

Theorem 3.7. Given that $\mathfrak{G}$ to be a setipiprant, the following $\mathfrak{NM}$ -polynomial of $\mathfrak{G}$.
$\mathfrak{NM}(\mathfrak{G}; g, h) = g^3h^4 + 2g^3h^5 + g^3h^7 + 5g^4h^5 + g^4h^6 + 3g^5h^5 + g^5h^6 + 3g^5h^7 + 4g^5h^8 + g^6h^7 + 3g^6h^8 + g^7h^7 + 2g^7h^8 + 6g^8h^8$

Theorem 3.8. If $\mathfrak{G}$ is a setipiprant, then that $\mathfrak{G}$′s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{\mathrm{M}_1}(\mathfrak{G}) = 412$
2. $\mathfrak{NM}_{\mathrm{M}_2}(\mathfrak{G}) = 1288$
3. $\mathfrak{NM}_{\mathrm{M}_2^m}(\mathfrak{G}) = 1.1312$
4. $\mathfrak{NM}_{\mathrm{GRI}}(\mathfrak{G}) = 1288$
5. $\mathfrak{NM}_{\mathrm{IRI}}(\mathfrak{G}) = 1.1312$
6. $\mathfrak{NM}_{\mathrm{SDI}}(\mathfrak{G}) = 71.381$
7. $\mathfrak{NM}_{\mathrm{HI}}(\mathfrak{G}) = 5.936$
8. $\mathfrak{NM}_{\mathrm{ISI}}(\mathfrak{G}) = 100.84$
9. $\mathfrak{NM}_{\mathrm{AZ}}(\mathfrak{G}) = 1705.1$
10. $\mathfrak{NM}_{\mathrm{ReZ}_1}(\mathfrak{G}) = 12.194$
11. $\mathfrak{NM}_{\mathrm{ReZ}_3}(\mathfrak{G}) = 17166$
12. $\mathfrak{NM}_{\mathrm{ABC}}(\mathfrak{G}) = 18.287$
13. $\mathfrak{NM}_{\mathrm{ABS}}(\mathfrak{G}) = 30.88$
14. $\mathfrak{NM}_{\mathrm{F}}(\mathfrak{G}) = 2641$
15. $\mathfrak{NM}_{\mathrm{SK}_2}(\mathfrak{G}) = 1312.5$
16. $\mathfrak{NM}_{\mathrm{RR}}(\mathfrak{G}) = 203.82$
17. $\mathfrak{NM}_{\mathrm{SI}}(\mathfrak{G}) = 9.9728$
18. $\mathfrak{NM}_{\mathrm{GA}_1}(\mathfrak{G}) = 34.416$
19. $\mathfrak{NM}_{\mathrm{AG}}(\mathfrak{G}) = 33.6$

Theorem 3.9. Given that $\mathfrak{G}$ to be a bedoradrine , the following $\mathfrak{NM}$ -polynomial of $\mathfrak{G}$. $\mathfrak{NM}$ (G; g, h) = $g^2h^3 + 3g^3h^5 + 3g^3h^6 + 5g^5h^5 + 8g^5h^6 + 4g^5h^7 + 2g^6h^6 + 6g^6h^7 + g^7h^7$

Theorem 3.10. If $\mathfrak{G}$ is a bedoradrine, then that $\mathfrak{G}$′s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 358$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 983$
3. $\mathfrak{NM}_{M_2^m}(\mathfrak{G}) = 1.3331$
4. $\mathfrak{NM}_{GRI}(\mathfrak{G})^{2} = 983$
5. $\mathfrak{NM}_{IRI}(\mathfrak{G}) = 1.3331$
6. $\mathfrak{NM}_{SDI}(\mathfrak{G}) = 69.333$
7. $\mathfrak{NM}_{HI}(\mathfrak{G}) = 6.3371$
8. $\mathfrak{NM}_{ISI}(\mathfrak{G}) = 87.694$
9. $\mathfrak{NM}_{AZ}(\mathfrak{G}) = 1221.6$
10. $\mathfrak{NM}_{ReZ_1}(\mathfrak{G}) = 13.048$
11. $\mathfrak{NM}_{ReZ_3}(\mathfrak{G}) = 11272$
12. $\mathfrak{NM}_{ABC}(\mathfrak{G}) = 18.444$
13. $\mathfrak{NM}_{ABS}(\mathfrak{G}) = 29.649$
14. $\mathfrak{NM}_{F}(\mathfrak{G}) = 2036$
15. $\mathfrak{NM}_{SK_2}(\mathfrak{G}) = 1000.5$
16. $\mathfrak{NM}_{RR}(\mathfrak{G}) = 177.15$
17. $\mathfrak{NM}_{SI}(\mathfrak{G}) = 10.165$
18. $\mathfrak{NM}_{GA_1}(\mathfrak{G}) = 33.409$
19. $\mathfrak{NM}_{AG}(\mathfrak{G}) = 32.606$

Theorem 3.11. Given that $\mathfrak{G}$ to be a toreforant, the following $\mathfrak{NM}$ -polynomial of $\mathfrak{G}$. $\mathfrak{NM}$ ($\mathfrak{G}$; g, h) = $2g^3h^5 + 2g^3h^6 + g^4h^4 + 2g^4h^5 + 5g^5h^5 + 7g^5h^6 + g^5h^8 + 3g^6h^6 + 4g^6h^7 + 3g^6h^8 + 2g^7h^8$

Theorem 3.12. If $\mathfrak{G}$ is a toreforant, then that $\mathfrak{G}$′s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 360$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 1029$
3. $\mathfrak{NM}_{M_2^m}(\mathfrak{G}) = 1.1421$
4. $\mathfrak{NM}_{GRI}(\mathfrak{G})^{2} = 1029$

5. $\mathfrak{NM}_{\mathrm{IRI}}(\mathfrak{G}) = 1.1421$
6. $\mathfrak{NM}_{\mathrm{SDI}}(\mathfrak{G}) = 66.473$
7. $\mathfrak{NM}_{\mathrm{HI}}(\mathfrak{G}) = 5.8761$
8. $\mathfrak{NM}_{\mathrm{ISI}}(\mathfrak{G}) = 88.538$
9. $\mathfrak{NM}_{\mathrm{AZ}}(\mathfrak{G}) = 1305.3$
10. $\mathfrak{NM}_{\mathrm{ReZ}_1}(\mathfrak{G}) = 12.007$
11. $\mathfrak{NM}_{\mathrm{ReZ}_3}(\mathfrak{G}) = 12308$
12. $\mathfrak{NM}_{\mathrm{ABC}}(\mathfrak{G}) = 17.586$
13. $\mathfrak{NM}_{\mathrm{ABS}}(\mathfrak{G}) = 28.907$
14. $\mathfrak{NM}_{\mathrm{F}}(\mathfrak{G}) = 2120$
15. $\mathfrak{NM}_{\mathrm{SK}_2}(\mathfrak{G}) = 1044.5$
16. $\mathfrak{NM}_{\mathrm{RR}}(\mathfrak{G}) = 178.51$
17. $\mathfrak{NM}_{\mathrm{SI}}(\mathfrak{G}) = 9.6568$
18. $\mathfrak{NM}_{\mathrm{GA}_1}(\mathfrak{G}) = 32.304$
19. $\mathfrak{NM}_{\mathrm{AG}}(\mathfrak{G}) = 31.707$

The aforementioned findings are obtained using the partition table-2 and the conditions of the $\mathfrak{NM}$ -Polynomial with its derivatives[11, 8, 20, 15].

4. Neighbourhood Degree Sum-Based Entropy Measures of anti-asthmatic drugs .

Theorem 4.1. If $\mathfrak{G}$ is a isoproterenol, then $\mathfrak{NM}$ - measures of entropy are given as follows [1, 13, 14].

1. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_1} = 2.691$
2. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_2} = 2.6377$
3. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_2^m} = 2.6223$
4. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{GRI}} = 2.6377$
5. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{IRI}} = 2.6223$
6. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SDD}} = 2.7043$
7. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{HI}} = 2.6885$
8. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ISI}} = 2.6868$
9. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AZ}} = 4.4163$
10. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_1} = 2.6848$
11. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_3} = 2.5696$

12. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABC}} = 2.7047$
13. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABS}} = 2.3269$
14. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{F}} = 2.6481$
15. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SK}_2} = 5.7008$
16. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{RR}} = 2.6889$
17. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SI}} = 2.7033$
18. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AG}_1} = 2.7078$
19. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{GA}} = 2.7079$

Theorem 4.2. If $\mathfrak{G}$ is a terbutaline then $\mathfrak{NM}$ - measures of entropy are given as follows [1, 13, 14].

1. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_1} = 2.7735$
2. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_2} = 2.7214$
3. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_2^{\mathrm{m}}} = 2.7158$
4. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{GRI}}\mathrm{N}\overset{2}{\mathrm{M}}\mathrm{ENT}_{\mathrm{GRI}} = 2.7214$
5. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{IRI}} = 2.7158$
6. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SDD}} = 2.7708$
7. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{HI}} = 2.7602$
8. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ISI}} = 2.7576$
9. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AZ}} = 4.5119$
10. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_1} = 2.7564$
11. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_3} = 2.6673$
12. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABC}} = 2.7701$
13. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABS}} = 2.7724$
14. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{F}} = 2.7306$
15. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SK}_2} = 3.224$
16. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{RR}} = 2.7591$
17. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SI}} = 2.7696$
18. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AG}_1} = 2.7724$
19. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{GA}} = 2.7725$

Theorem 4.3. If $\mathfrak{G}$ is a , pranlukast then $\mathfrak{NM}$ - measures of entropy are given as follows [1, 13, 14].

1. $\mathfrak{NM}\mathrm{ENT}_{M_1} = 3.6702$
2. $\mathfrak{NM}\mathrm{ENT}_{M_2} = 3.6137$
3. $\mathfrak{NM}\mathrm{ENT}_{M_2^m} = 3.617$
4. $\mathfrak{NM}\mathrm{ENT}_{GRI} = 3.6137$
5. $\mathfrak{NM}\mathrm{ENT}_{IRI} = 3.617$
6. $\mathfrak{NM}\mathrm{ENT}_{SDD} = 3.6876$
7. $\mathfrak{NM}\mathrm{ENT}_{HI} = 3.6929$
8. $\mathfrak{NM}\mathrm{ENT}_{ISI} = 3.6693$
9. $\mathfrak{NM}\mathrm{ENT}_{AZ} = 5.2892$
10. $\mathfrak{NM}\mathrm{ENT}_{ReZ_1} = 3.6698$
11. $\mathfrak{NM}\mathrm{ENT}_{ReZ_3} = 3.5298$
12. $\mathfrak{NM}\mathrm{ENT}_{ABC} = 3.6857$
13. $\mathfrak{NM}\mathrm{ENT}_{ABS} = 3.6842$
14. $\mathfrak{NM}\mathrm{ENT}_{F} = 3.6162$
15. $\mathfrak{NM}\mathrm{ENT}_{SK_2} = 4.009$
16. $\mathfrak{NM}\mathrm{ENT}_{RR} = 3.6696$
17. $\mathfrak{NM}\mathrm{ENT}_{SI} = 3.6849$
18. $\mathfrak{NM}\mathrm{ENT}_{AG_1} = 3.6894$
19. $\mathfrak{NM}\mathrm{ENT}_{GA} = 3.6882$

Theorem 4.4. If $\mathfrak{G}$ is a setipiprant then $\mathfrak{NM}$ - measures of entropy are given as follows [1, 13, 14].

1. $\mathfrak{NM}\mathrm{ENT}_{M_1} = 3.5$
2. $\mathfrak{NM}\mathrm{ENT}_{M_2} = 3.4258$
3. $\mathfrak{NM}\mathrm{ENT}_{M_2^m} = 3.4155$
4. $\mathfrak{NM}\mathrm{ENT}_{GRI} = 3.4258$
5. $\mathfrak{NM}\mathrm{ENT}_{IRI} = 3.4155$
6. $\mathfrak{NM}\mathrm{ENT}_{SDD} = 3.5311$
7. $\mathfrak{NM}\mathrm{ENT}_{HI} = 3.4969$
8. $\mathfrak{NM}\mathrm{ENT}_{ISI} = 3.4971$

9. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AZ}}$ = 4.8422
10. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_1}$ = 3.5034
11. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_3}$ = 3.3279
12. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABC}}$ = 3.5254
13. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABS}}$ = 3.5259
14. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{F}}$ = 3.3666
15. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SK}_2}$ =6.8929
16. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{RR}}$= 3.499
17. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SI}}$= 3.519
18. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AG}_1}$ = 3.5282
19. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{GA}}$= 3.5243

Theorem 4.5. If $\mathfrak{G}$ is a bedoradrine then $\mathfrak{NM}$ - measures of entropy are given as follows [1, 13, 14].

1. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_1}$ = 3.5035
2. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_2}$ = 3.4362
3. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{M}_2^m}$= 3.3568
4. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{GRI}}$ = 3.4362
5. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{IRI}}$ =3.3568
6. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SDD}}$ = 3.494
7. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{HI}}$ = 3.4711
8. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ISI}}$ = 3.4767
9. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AZ}}$ = 5.205
10. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_1}$= 3.4659
11. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ReZ}_3}$ = 3.3837
12. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABC}}$ = 3.493
13. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{ABS}}$ = 3.4959
14. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{F}}$ = 3.4457
15. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SK}_2}$ =3.8808
16. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{RR}}$= 3.4783
17. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{SI}}$= 3.491
18. $\mathfrak{NM}\mathrm{ENT}_{\mathrm{AG}_1}$= 3.4964

19. $\mathfrak{NM}\mathrm{ENT}_{GA} = 3.4963$

Theorem 4.6. If $\mathfrak{G}$ is a toreforant then $\mathfrak{NM}$ - measures of entropy are given as follows [1, 13, 14].

1. $\mathfrak{NM}\mathrm{ENT}_{M_1} = 3.7278$
2. $\mathfrak{NM}\mathrm{ENT}_{M_2} = 3.8596$
3. $\mathfrak{NM}\mathrm{ENT}_{M_2^m} = 3.1607$
4. $\mathfrak{NM}\mathrm{ENT}_{GRI} = 3.8596$
5. $\mathfrak{NM}\mathrm{ENT}_{IRI} = 3.1607$
6. $\mathfrak{NM}\mathrm{ENT}_{SDD} = 3.5283$
7. $\mathfrak{NM}\mathrm{ENT}_{HI} = 3.3022$
8. $\mathfrak{NM}\mathrm{ENT}_{ISI} = 3.5762$
9. $\mathfrak{NM}\mathrm{ENT}_{AZ} = 5.3788$
10. $\mathfrak{NM}\mathrm{ENT}_{ReZ_1} = 3.3556$
11. $\mathfrak{NM}\mathrm{ENT}_{ReZ_3} = 4.1708$
12. $\mathfrak{NM}\mathrm{ENT}_{ABC} = 3.4042$
13. $\mathfrak{NM}\mathrm{ENT}_{ABS} = 3.4575$
14. $\mathfrak{NM}\mathrm{ENT}_{F} = 3.9415$
15. $\mathfrak{NM}\mathrm{ENT}_{SK_2} = 4.2029$
16. $\mathfrak{NM}\mathrm{ENT}_{RR} = 3.65223$
17. $\mathfrak{NM}\mathrm{ENT}_{SI} = 3.3512$
18. $\mathfrak{NM}\mathrm{ENT}_{AG_1} = 3.4658$
19. $\mathfrak{NM}\mathrm{ENT}_{GA} = 3.465$

4. Comparative Analysis

The three-dimensional graphs derived from Theorems 3 and 4 that illustrate the analytical equations for the neighbourhood degree sum-based indices are shown in this section. The reader will find it easier to comprehend and grasp how the indices operate in relation to the variables that form the molecular structure thanks to these illustrations. The differences between the indices and the chemical structure are graphically represented in these comparison charts. Tables 8–11 display the calculated numerical values for the indices. To aid readers in understanding the numerical data, Figure 3 and 4 present them as three-dimensional graphs.

Drugs	$\mathfrak{NM}_{M1}$	$\mathfrak{NM}_{M2}$	$\mathfrak{NM}^{m}{}_{2}M$	$\mathfrak{NM}GRI$	$\mathfrak{NM}IRI$	$\mathfrak{NM}SDD$	$\mathfrak{NM}_{HI}$	$\mathfrak{NM}ISI$	$\mathfrak{NM}_{AZ}$
Drug 1	154	399	0.66175	399	0.66175	31.945	3.0316	37.484	484.6
Drug 2	168	444	0.64365	444	0.64365	33.488	3.1232	41.2	544.47
Drug 3	438	1226	1.5178	1226	1.5178	82.676	7.3359	107.82	1548.6
Drug 4	412	1288	1.1312	1288	1.1312	71.381	5.936	100.84	1705.1
Drug 5	358	983	1.3331	983	1.3331	69.333	6.3371	87.694	1221.6
Drug 6	360	1029	1.1421	1029	1.1421	66.473	5.8761	88.538	1305.3

Table 8. Comparison Table for $\mathfrak{NM}$ -values

$\mathfrak{NM}ReZ_{1}$	$\mathfrak{NM}_{Rez_3}$	$\mathfrak{NM}ABC$	$\mathfrak{NM}ABS$	$\mathfrak{NM}_{F}$	$\mathfrak{NM}_{SK2}$	$\mathfrak{NM}_{RR}$	$\mathfrak{NM}_{\chi}$	$\mathfrak{NM}_{AG1}$	$\mathfrak{NM}_{GA}$
6.2786	4370	8.5924	13.394	836	408.5	75.959	4.7455	15.237	14.774
6.4119	4890	9.0326	14.35	918	451.5	83.188	4.9831	16.183	15.823
15.431	14446	22.201	35.818	2526	1244.5	217.28	12.20	40.33	39.681

							3		
12.194	17166	18.287	30.88	2641	1312.5	203.82	9.9728	34.416	33.6
13.048	11272	18.444	29.649	2036	1000.5	177.15	10.165	33.409	32.606
12.007	12308	17.586	28.907	2120	1044.5	178.51	9.6568	32.304	31.707

Table 9. Comparison Table for $\mathfrak{NM}$ -values

Drugs	$\mathfrak{NM}_{M1}$	$\mathfrak{NM}_{M2}$	$\mathfrak{NM}^{m}_{2}M$	$\mathfrak{NM}GRI$	$\mathfrak{NM}IRI$	$\mathfrak{NM}SDD$	$\mathfrak{NM}_{HI}$	$\mathfrak{NM}ISI$	$\mathfrak{NM}_{AZ}$
Drug 1	2.691	2.6377	2.6223	2.6377	2.6223	2.7043	2.6885	2.6868	4.4163
Drug 2	2.7735	2.7214	2.7158	2.7214	2.7158	2.7708	2.7602	2.7576	4.5119
Drug 3	3.6702	3.6137	3.617	3.6137	3.617	3.6876	3.6929	3.6693	5.2892
Drug 4	3.5	3.4258	3.4155	3.4258	3.4155	3.5311	3.4969	3.4971	4.8422
Drug 5	3.5035	3.4362	3.3568	3.4362	3.3568	3.494	3.4711	3.4767	5.205
Drug 6	3.7278	3.8596	3.1607	3.8596	3.1607	3.5283	3.3022	3.5762	5.3788

Table 10. Comparison Table for Entropy-values

$\mathfrak{NM}ReZ_1$	$\mathfrak{NM}_{Rez_3}$	$\mathfrak{NM}ABC$	$\mathfrak{NM}ABS$	$\mathfrak{NM}_F$	$\mathfrak{NM}_{SK}2$	$\mathfrak{NM}_{RR}$	$\mathfrak{NM}_\chi$	$\mathfrak{NM}_{AG}1$	$\mathfrak{NM}_{GA}$
2.6848	2.5696	2.7047	2.3269	2.6481	5.7008	2.6889	2.7033	2.7078	2.7079
2.7564	2.6673	2.7701	2.7724	2.7306	3.224	2.7591	2.7696	2.7724	2.7725
3.6698	3.5298	3.6857	3.6842	3.6162	4.009	3.6696	3.6849	3.6894	3.6882
3.5034	3.3279	3.5254	3.5259	3.3666	6.8929	3.499	3.519	3.5282	3.5243
3.4659	3.3837	3.493	3.4959	3.4457	3.8808	3.4783	3.491	3.4964	3.4963
3.3556	4.1708	3.4042	3.4575	3.941	4.2029	3.6522	3.351	3.4658	3.4653

				5			2		

Table 11. Comparison Table for Entropy-values

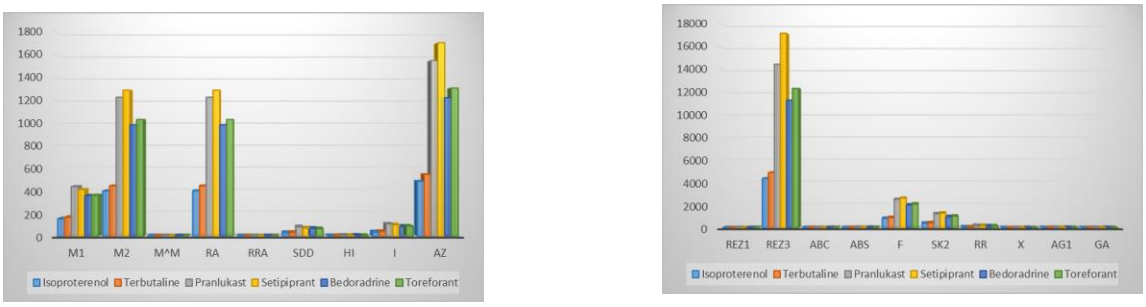

Figure 2: 3D plots for Table 8 and 9

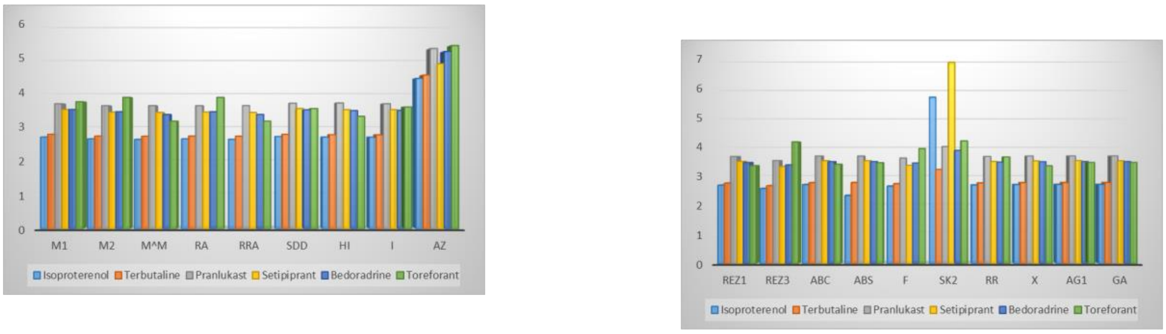

Figure 3: 3D plots for Table 10 and 11

5. Conclusions

This article computes the M-Polynomial to get the closed-form analytical formulas for the neighbourhood sum degree-based indices for the 6 different anti-asthmatic drugs such as isoproterenol, terbutaline, pranlukast, setipiprant, bedoradrine, toreforant using a set of 19 degree - based topological indices. The results are shown as separate three-dimensional plots and comparison plots to aid in the comprehension of the mathematical expressions. For all the above drugs, Neighbourhood Degree Sum-Based Entropy Measures are computed. This finding will provide new perspectives for future research on topological indices for these drugs

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Conflicts of Interest

The authors declare that none of the work reported in this study could have been influenced by any known competing financial interests or personal relationships.

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