International Journal of Applied Mathematics

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

NUMERICAL DESCRIPTOR COMPUTATION OF ALOPECIA DRUGS USING COM – POLYNOMIAL

S Shenbaga Devi[1,2] and S Dhanalakshmi[2,*]

[1] *Department of Mathematics, Loyola ICAM College of Engineering and Technology, Loyola Campus, Nungambakkam, Chennai 600 034, India.*

[2] *Department of Mathematics, SRM Institute of Science and Technology, Ramapuram Campus, Chennai 600 089, India.*

[1] *ss1338@srmist.edu.in*

[2,*] *Corresponding author: dhanalas1@srmist.edu.in*

Abstract. A molecular graph can be represented numerically using topological indices to support thorough investigation of the medications. Several medications are used to project their physicochemical properties. Alopecia, including alopecia areata, is quite prevalent in India, impacting one million individuals. Alopecia may be transient or enduring, localized or widespread, and is attributable to various factors, including genetic predisposition, hormonal fluctuations, medical disorders, or stress. The derivation of CoM – polynomial and few degree-based topological coindices for the drugs in the treatment of alopecia like Minoxidil, Finasteride, Dutasteride, Biotin, Triamcinolone, Spironolactone, Ritlecitinib, Baricitinib, Dithranol and Sulfasalazine are shown in this work. This is especially beneficial in developing nations where laboratory resources may be constrained.

Keywords: Topological coindices; CoM – Polynomial; Alopecia treatment;

1. INTRODUCTION

Alopecia areata is a disorder that is characterized by the presence of hair follicles being attacked by the immune system, which ultimately leads to hair loss. Hair follicles are the integumentary structures responsible for hair formation. Alopecia areata often impacts the scalp and facial regions, although hair loss can occur on any body part. Hair loss generally occurs in small, circular patches approximately the size of a quarter; however, in certain instances, it may be more extensive. The progression of alopecia areata differs among individuals. Some individuals experience recurrent episodes of hair loss throughout their life, whereas others encounter a singular occurrence.

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Recovery is also uncertain, as some individuals get complete hair regrowth while others do not. Alopecia areata has no cure; however, therapies exist that expedite hair regrowth. Resources are available to assist individuals in managing hair loss. Both men and women can contract it, and it impacts all racial and ethnic demographics. It may commence at any age, however the majority of individuals experience it throughout their teenage years, twenties, or thirties. In youngsters under the age of 10, it typically manifests as more extensive and progressive. A familial predisposition to the disease may elevate our danger, although for numerous individuals, there is an absence of familial history. Researchers have associated several genes with the condition, indicating that genetics contribute to alopecia areata. A number of the identified genes are crucial for the operation of the immune system. Individuals with specific autoimmune disorders, such psoriasis, thyroid disease, or vitiligo, exhibit a heightened susceptibility to alopecia areata. Emotional stress or sickness may precipitate alopecia areata in predisposed individuals; but, in the majority of instances, no discernible trigger is evident [1].

Medications and other therapies assist in managing hair loss, although they do not provide a cure for the condition. Alopecia areata totalis and alopecia areata universalis are more severe conditions and exhibit a diminished likelihood of responding to treatment. In instances of moderate alopecia areata, characterized by minimal hair loss, regrowth may occur spontaneously without intervention, but hair loss frequently reappears. Conventional therapies for alopecia areata involve the administration of steroids, either via injection or topical application (creams or liquids) to the affected areas of hair loss. Steroids inhibit the immune cells that target hair follicles, facilitating hair regrowth. An alternative method involves the topical application of an irritant like squaric acid, producing a rash akin to that of poison ivy. The resultant inflammation appears to undermine the immune system's assault on the hair follicles. Alopecia drug modeling is important because it helps scientists understand how potential drug compounds interact with biological targets that are responsible for hair growth. This lets them come up with better and more targeted treatments. It also speeds up the process of finding new drugs by using computer simulations to predict their effectiveness, safety, and pharmacological properties. This cuts down on the costs and time needed for experiments. This treatment frequently induces discomfort in the patient, resulting in erythema

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

and pruritus. [2] This analysis encompasses the pharmacological interventions utilized for the purpose of alopecia management, including Minoxidil, Finasteride, Dutasteride, Biotin, Triamcinolone, Spironolactone, Ritlecitinib, Baricitinib, Dithranol, and Sulfasalazine.

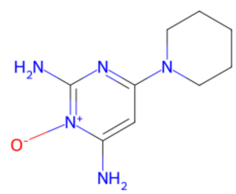
The molecular formula of Minoxidil is $C_9H_{15}N_5O$. A vasodilator, minoxidil increases the amount of blood that flows to hair follicles, it allows the anagen phase of the hair growth cycle to last longer and perhaps increasing follicular size. Regular use can help to slow down hair loss, especially in the first to moderate phases. The molecular formula for Finasteride is $C_{23}H_{36}N_2O_2$. Finasteride treats androgenetic alopecia from its fundamental source. Finasteride lessens the activity of the enzyme 5-alpha reductase, which is responsible for the conversion of testosterone into dihydrotestosterone (DHT), an essential hormone that is accountable for the atrophy of hair follicles in androgenetic alopecia. The molecular formula for Dutasteride $C_{27}H_{30}F_6N_2O_2$. While Finasteride just inhibits Type II 5-alpha reductase enzymes, Dutasteride inhibits Type I and Type II 5-alpha reductase enzymes. Unlike Finasteride, this causes DHT levels to drop over 90% instead of about 60–70%. The molecular formula for Biotin is $C_{10}H_{16}N_2O_3S$. Dermal rashes, brittle nails, and hair thinning could all follow from biotin insufficiency. For those with low biotin levels, biotin supplements can bring about hair growth. The molecular formula for Triamcinolone is $C_{21}H_{27}FO_6$. Strong anti-inflammatory effect of triamcinolone helps the immune system in autoimmune alopecia to calm down. When alopecia areata strikes, the immune system assaults hair follicles; triamcinolone can stop this assault and promote regrowth. Usually as Triamcinolone acetonide, it stimulates hair growth via injection into the affected areas of the scalp. It is usually beneficial in localized alopecia and produces noticeable results in 4 to 8 weeks. The molecular formula for Spironolactone $C_{24}H_{32}O_4S$. Specifically, testosterone and dihydrotestosterone (DHT), spironolactone reduces androgen production and blocks androgen receptors. This helps female pattern hair loss (FPHL), in which raised androgens reduce hair follicles. The molecular formula for Ritlecitinib is $C_{15}H_{19}N_5O$. Authorized for severe alopecia areata in those 12 years of age and above is ritlecitinib.
One of the first oral treatments approved specifically for this condition, which had limited focused options before. The molecular formula for Baricitinib is $C_{16}H_{17}N_7O_2S$. One of the first oral

Volume 38 No. 9s, 2025

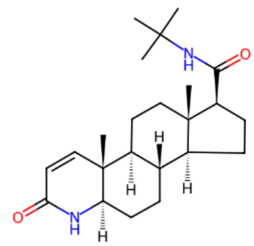
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

treatments approved specifically for this condition, which had limited focused options before. Approved as the first systematic treatment for severe alopecia areata in adults in 2022, baricitinib. Baricitinib works by blocking JAK1 and JAK2, therefore reducing the inflammatory impulses that cause follicle destruction. It promotes regeneration both in acute and chronic conditions. The molecular formula for Dithranol is $C_{14}H_{10}O_3$. Dithranol causes minor cutaneous irritation that seems to either direct or change the localized immune response aimed at hair follicles in alopecia areata. Especially when taken early in the course of the disease, dithranol has shown effectiveness in encouraging hair regeneration in patchy alopecia areata. The molecular formula for Sulfasalazine is $C_{18}H_{14}N_4O_5S$. Those who do not respond to first-line treatments can benefit from sulfasalazine. Studies show that in some people with patchy alopecia areata, sulfasalazine could help either partially or totally regenerate hair [3].

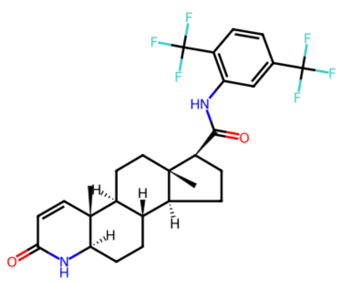
Graph theory provides a useful tool, the topological index, for linking in conjunction with their molecular structure, the physicochemical properties of chemical substances. There is a unique set of real numbers that defines their topology for every set of all conceivable molecular graphs, which are simple connected graphs; this set is denoted as the topological index and does not change for isomorphic graphs. Graph polynomial is the graph invariant having a poisson value. Investigated in algebraic graph theory are invariants of this type [4 – 6]. The Hosoya polynomial is an essential integral part of the study of distance-based topological indices [7]. One of the two recently provided new instruments, Deutsch and Klavžar were the ones who initially introduced the M-polynomial [8]. Essential for starting closed procedures of various indices for topology based on degrees, Mondal et al. developed the NM-polynomial [9]. M-Polynomial extended for non-adjacent pair of vertices by Kirmani et al. will be relevant in 2022 is CoM - Polynomial. The time-consuming computation of several kinds of graph coindices has to be accelerated. This serves as a driving force behind our efforts to build polynomials that are dependent on pairs of vertices of chemical molecules that are not adjacents. The topological coindices are derived from the generalized version of the CoM – polynomial, which is the source data. This article presents the computation of CoM-polynomial for the ten drugs which are used in the treatment of alopecia. Also, we derive the respective degree based topological coindices [10 – 13, 22, 23]. Figure 1 shows the 10 drugs which are used in the treatment of alopecia.



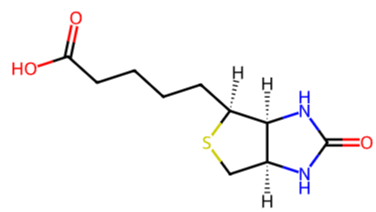
1(a)



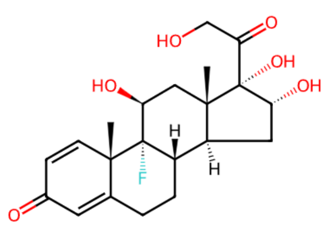
1(b)



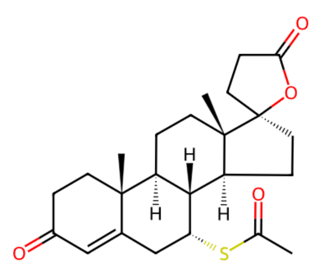
1(c)



1(d)



1(e)

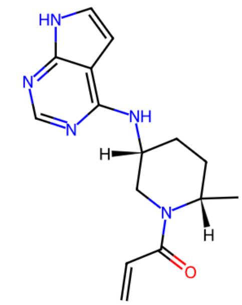


1(f)

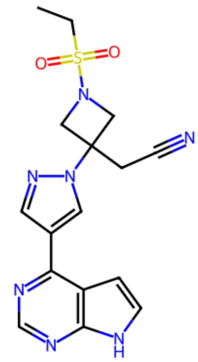
International Journal of Applied Mathematics

Volume 38 No. 9s, 2025

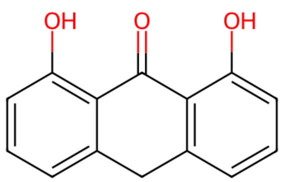
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)



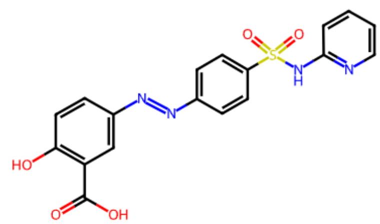
1(g)



1(h)



1(i)



1(j)

***Figure 1**: 1(a) Minoxidil, 1(b) Finasteride, 1 (c) Dutasteride 1(d) Biotin 1(e) Triamcinolone 1(f) Spironolactone 1(g) Ritlecitinib, 1(h) Baricitinib 1(i) Dithranol 1(j)Sulfasalazine*

2. Methodology

Suppose that, T be a connected simple graph, with $V(T)$ as the vertex set, $E(T)$ as the edge set and $d_p = d(p)$ be number of vertices adjacent to the vertex p is called the degree of any vertex p.

The CoM – polynomial of T [10] is defined as

$$CoM(T;r,s) = \overline{M}(T;r,s) = \sum_{i\leq j} \overline{m}_{ij} r^i s^j$$

Where $\overline{m}_{ij}$ denotes the number of edges $xy \notin E(T), d(x) = i, d(y) = j$.

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

This polynomial helps figure out how changes in structure affect biological activity, which makes it possible to accurately predict how well a drug will work and improve compounds for treating alopecia.

The subsequent operators are employed in the derivation of degree-based topological indices obtained from the CoM polynomial by treating a polynomial as $l(r,s)$.

$$D_r = r\frac{\partial l(r,s)}{\partial r}$$

$$D_s = s\frac{\partial l(r,s)}{\partial s}$$

$$S_r = \int_0^r \frac{l(t,s)}{t}dt$$

$$S_s = \int_0^r \frac{l(r,t)}{t}dt$$

$$Jl(r,s) = l(r,r).$$

The degree based topological coindices of the graph T, which are indicated by the notation DBTCI(T), are defined as the sum of $l(r,s)\ \forall\ \ rs \notin E(T)$. Using the CoM polynomial, we were able to generate a few indices, and Table 1 presents a few DBTCI along with their relationship to the CoM polynomial of T.

Table 1: Relation between topological indices and CoM - polynomial

DBTCI	$\boldsymbol{g(r,s)}$	**Derivation from $\boldsymbol{CoM(T;r,s)}$**
First Zagreb coindex $\overline{M_1}(T)$ [14]	d_r+d_s	$(D_r + D_s)\big(CoM(T;r,s)\big)\vert_{r=s=1}$
Second Zagreb coindex $\overline{M_2}(T)$ [14]	d_rd_s	$(D_rD_s)\big(CoM(T;r,s)\big)\vert_{r=s=1}$
Second modified Zagreb coindex $\overline{MM_2}(T)$ [15]	$\frac{1}{d_rd_s}$	$(S_rS_s)\big(CoM(T;r,s)\big)\vert_{r=s=1}$

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Redefined Zagreb coindex $\overline{ReZ}(T)$ [16]	$(d_r d_s)(d_r+d_s)$	$(D_r D_s)(D_r + D_s)\big(CoM(T;r,s)\big)\vert_{r=s=1}$
Symmetric Division coindex $\overline{SDD}(T)$ [17]	$\frac{\min(d_r,d_s)}{\max(d_r,d_s)} + \frac{\max(d_r,d_s)}{\min(d_r,d_s)}$	$(D_r S_s + D_s S_r)\big(CoM(T;r,s)\big)\vert_{r=s=1}$
Harmonic coindex $\overline{H}(T)$ [18]	$\frac{2}{(d_r+d_s)}$	$2S_r J\big(CoM(T;r,s)\big)\vert_{r=s=1}$
Inverse Sum coindex $\overline{I}(T)$ [19]	$\frac{d_r d_s}{d_r+d_s}$	$S_r J(D_r D_s)\big(CoM(T;r,s)\big)\vert_{r=s=1}$
Forgotten coindex $\overline{F}(T)$ [20]	$d_r^2 + d_s^2$	$(D_r^2 + D_s^2)\,\big(CoM(T;r,s)\big)\vert_{r=s=1}$

We possess the subsequent assertion for a connected graph H comprising n vertices [21].

- If $i = j$, then $\overline{m}_{ij} = \left|\overline{E}_{ij}\right| = \frac{n_i(n_i-1)}{2} - m_{ii}$
- If $i \leq j$, then $\overline{m}_{ij} = \left|\overline{E}_{ij}\right| = n_i n_j - m_{ij}$

3. Results and discussion

Theorem 3.1. The CoM – polynomial of the molecular graph of the drug Minoxidil (A) is

$$CoM(A;r,s) = 12rs^3 + 17r^2s^2 + 29r^2s^3 + 7r^3s^3.$$

Proof:

Let A be the molecular graph of the drug Minoxidil with $|V(A)| = 15$ and $|E(A)| = 16$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the minoxidil molecular graph can be partitioned as illustrated in Tables 2 & 3.

TABLE .2. *Partition of vertices*

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$n_i = \|V_i\|$	n_1	n_2	n_3
Number of vertices of degree i	3	7	5

TABLE .3. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{13}	m_{22}	m_{23}	m_{33}
Number of edges with i & j as the adjacent vertices	3	4	6	3

We get

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 12$$

$$\overline{m_{22}} = \frac{n_2(n_2-1)}{2} - m_{22} = 17$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 29$$

$$\overline{m_{33}} = \frac{n_3(n_3-1)}{2} - m_{33} = 7$$

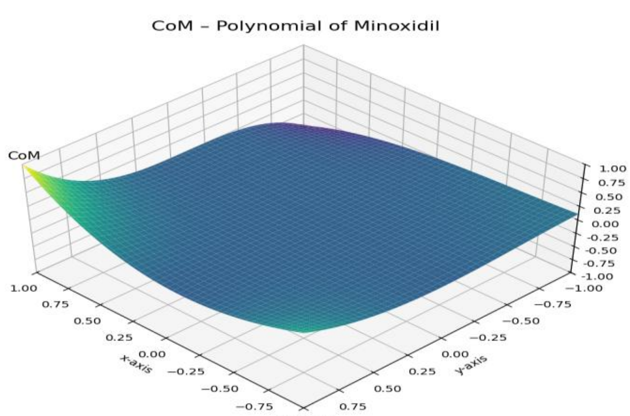
The CoM – polynomial of the graph A is

$$CoM(A; r, s) = \sum_{i \leq j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{13}} r^1 s^3 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{33}} r^3 s^3$$

$$= 12 r^1 s^3 + 17 r^2 s^2 + 29 r^2 s^3 + 7 r^3 s^3.$$

Hence, the proof.



International Journal of Applied Mathematics

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Figure 2: CoM – Polynomial of Minoxidil

Proposition: 3.1

The degree based topological coindices of A is

i. $\overline{M_1}(A) = 303$
ii. $\overline{M_2}(A) = 341$
iii. $\overline{MM_2}(A) = 13.8611$
iv. $\overline{ReZ}(A) = 1664$
v. $\overline{SDD}(A) = 150.8333$
vi. $\overline{H}(A) = 28.4333$
vii. $\overline{I}(A) = 71.3$
viii. $\overline{F}(A) = 759$

Proof: We use $CoM(A; r, s) = 12r^1s^3 + 17r^2s^2 + 29r^2s^3 + 7r^3s^3$ to arrive at the following conclusions:

$$D_r = 12r^1s^3 + 34r^2s^2 + 58r^2s^3 + 21r^3s^3$$

$$D_s = 36r^1s^3 + 34r^2s^2 + 87r^2s^3 + 21r^3s^3$$

$$D_r + D_s = 48r^1s^3 + 68r^2s^2 + 145r^2s^3 + 42r^3s^3$$

$$D_rD_s = 36r^1s^3 + 68r^2s^2 + 174r^2s^3 + 63r^3s^3$$

$$D_r^2 = 12r^1s^3 + 68r^2s^2 + 116r^2s^3 + 63r^3s^3$$

$$D_s^2 = 108r^1s^3 + 68r^2s^2 + 261r^2s^3 + 63r^3s^3$$

$$D_r^2 + D_s^2 = 120r^1s^3 + 136r^2s^2 + 377r^2s^3 + 126r^3s^3$$

$$D_rD_s(D_r + D_s) = 144r^1s^3 + 272r^2s^2 + 870r^2s^3 + 378r^3s^3$$

$$S_r = 12r^1s^3 + \frac{17}{2}r^2s^2 + \frac{29}{2}r^2s^3 + \frac{7}{3}r^3s^3$$

$$S_s = 4r^1s^3 + \frac{17}{2}r^2s^2 + \frac{29}{3}r^2s^3 + \frac{7}{3}r^3s^3$$

$$S_rS_s = 4r^1s^3 + \frac{17}{4}r^2s^2 + \frac{29}{6}r^2s^3 + \frac{7}{9}r^3s^3$$

$$D_rS_s + D_sS_r = 40r^1s^3 + 34r^2s^2 + \frac{377}{6}r^2s^3 + 14r^3s^3$$

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$S_rJ = \frac{29}{4}r^4 + \frac{29}{5}r^5 + \frac{7}{6}r^6$$

$$S_rJ(D_rD_s) = \frac{104}{4}r^4 + \frac{174}{5}r^5 + \frac{63}{6}r^6$$

Thus, we get

i. $\overline{M_1}(A) = (D_r + D_s)\big(CoM(A;r,s)\big)|_{r=s=1} = 303$
ii. $\overline{M_2}(A) = (D_rD_s)\big(CoM(A;r,s)\big)|_{r=s=1} = 341$
iii. $\overline{MM_2}(A) = (S_rS_s)\big(CoM(A;r,s)\big)|_{r=s=1} = 13.8611$
iv. $\overline{ReZ}(A) = (D_rD_s)(D_r + D_s)\big(CoM(A;r,s)\big)|_{r=s=1} = 1664$
v. $\overline{SDD}(A) = (D_rS_s + D_sS_r)\big(CoM(A;r,s)\big)|_{r=s=1} = 150.8333$
vi. $\overline{H}(A) = 2S_rJ\big(CoM(A;r,s)\big)|_{r=s=1} = 28.4333$
vii. $\overline{I}(A) = S_rJ(D_rD_s)\big(CoM(A;r,s)\big)|_{r=s=1} = 71.3$
viii. $\overline{F}(A) = (D_r^2 + D_s^2)\ \big(CoM(A;r,s)\big)|_{r=s=1} = 759$

Hence, the proof.

Theorem 3.2. The CoM – polynomial of the molecular graph of the drug Finasteride (B) is

$$CoM(B;r,s) = 59rs^3 + 4rs^4 + 41r^2s^2 + 80r^2s^3 + 9r^2s^4 + 29r^3s^3.$$

Proof:

Let B be the molecular graph of the drug Finasteride with $|V(B)| = 27$ and $|E(B)| = 28$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the Finasteride molecular graph can be partitioned as illustrated in Tables 4 & 5.

TABLE .4. *Partition of vertices*

$n_i = \|V_i\|$	n_1	n_2	n_3	n_4
Number of vertices of degree i	7	10	9	1

TABLE .5. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Number of edges with i & j as the adjacent vertices	4	3	4	10	1	7

We get

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 59$$

$$\overline{m_{14}} = n_1 n_4 - m_{14} = 4$$

$$\overline{m_{22}} = \frac{n_2(n_2-1)}{2} - m_{22} = 41$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 80$$

$$\overline{m_{24}} = n_2 n_4 - m_{24} = 9$$

$$\overline{m_{33}} = \frac{n_3(n_3-1)}{2} - m_{33} = 29$$

The CoM – polynomial of the graph B is

$$CoM(B; r, s) = \sum_{i \leq j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{13}} r^1 s^3 + \overline{m_{14}} r^1 s^4 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{24}} r^2 s^4 + \overline{m_{33}} r^3 s^3$$

$$= 59 r^1 s^3 + 4 r^1 s^4 + 41 r^2 s^2 + 80 r^2 s^3 + 9 r^2 s^4 + 29 r^3 s^3.$$

Hence, the proof.

Received: August 07 2025

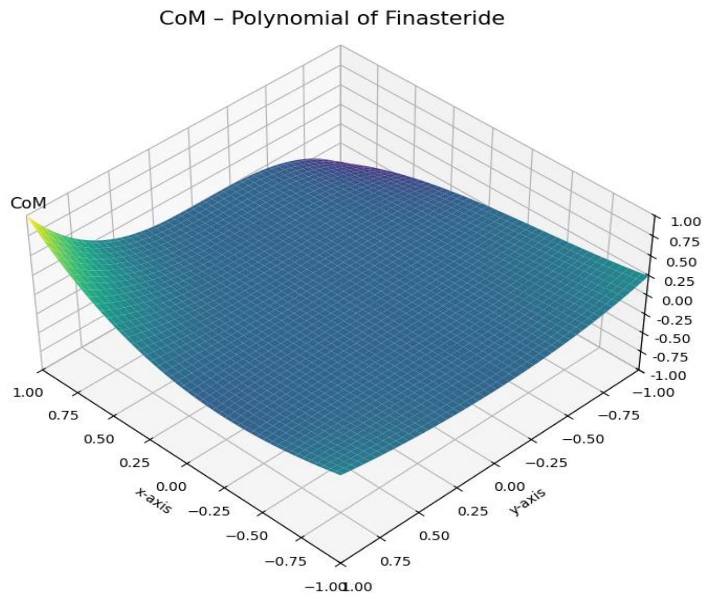


Figure 3: CoM – Polynomial of Finasteride

Proposition: 3.2

The degree based topological coindices of B is

i. $\overline{M_1}(B) = 1048$
ii. $\overline{M_2}(B) = 1170$
iii. $\overline{MM_2}(B) = 48.5972$
iv. $\overline{ReZ}(B) = 5842$
v. $\overline{SDD}(B) = 549.5$
vi. $\overline{H}(B) = 288.8$
vii. $\overline{I}(B) = 239.95$
viii. $\overline{F}(B) = 2728$

Proof: We use $CoM(B; r, s) = 59r^1s^3 + 4r^1s^4 + 41r^2s^2 + 80r^2s^3 + 9r^2s^4 + 29r^3s^3$ to arrive at the following conclusions:

$$D_r = 59r^1s^3 + 4r^1s^4 + 82r^2s^2 + 160r^2s^3 + 18r^2s^4 + 87r^3s^3$$

$$D_s = 177r^1s^3 + 16r^1s^4 + 82r^2s^2 + 240r^2s^3 + 36r^2s^4 + 87r^3s^3$$

$$D_r + D_s = 236r^1s^3 + 20r^1s^4 + 164r^2s^2 + 400r^2s^3 + 54r^2s^4 + 174r^3s^3$$

$$D_rD_s = 177r^1s^3 + 16r^1s^4 + 164r^2s^2 + 480r^2s^3 + 72r^2s^4 + 261r^3s^3$$

$$D_r^2 = 59r^1s^3 + 4r^1s^4 + 164r^2s^2 + 320r^2s^3 + 36r^2s^4 + 261r^3s^3$$

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$D_s^2 = 531r^1s^3 + 64r^1s^4 + 164r^2s^2 + 720r^2s^3 + 144r^2s^4 + 261r^3s^3$$

$$D_r^2 + D_s^2 = 590r^1s^3 + 68r^1s^4 + 328r^2s^2 + 1040r^2s^3 + 180r^2s^4 + 522r^3s^3$$

$$D_rD_s(D_r + D_s) = 708r^1s^3 + 80r^1s^4 + 656r^2s^2 + 2400r^2s^3 + 432r^2s^4 + 1566r^3s^3$$

$$S_r = 59r^1s^3 + 4r^1s^4 + \frac{41}{2}r^2s^2 + 40r^2s^3 + \frac{9}{2}r^2s^4 + \frac{29}{3}r^3s^3$$

$$S_s = \frac{59}{3}r^1s^3 + r^1s^4 + \frac{41}{2}r^2s^2 + \frac{80}{3}r^2s^3 + \frac{9}{4}r^2s^4 + \frac{29}{3}r^3s^3$$

$$S_rS_s = \frac{59}{3}r^1s^3 + r^1s^4 + \frac{41}{4}r^2s^2 + \frac{80}{6}r^2s^3 + \frac{9}{8}r^2s^4 + \frac{29}{9}r^3s^3$$

$$D_rS_s + D_sS_r = \frac{590}{3}r^1s^3 + 17r^1s^4 + 82r^2s^2 + \frac{520}{3}r^2s^3 + \frac{45}{2}r^2s^4 + 58r^3s^3$$

$$S_rJ = \frac{100}{4}r^4 + \frac{84}{5}r^5 + \frac{38}{6}r^6$$

$$S_rJ(D_rD_s) = \frac{341}{4}r^4 + \frac{496}{5}r^5 + \frac{333}{6}r^6$$

Thus, we get

i. $\overline{M_1}(B) = (D_r + D_s)\big(CoM(B;r,s)\big)|_{r=s=1} = 1048$
ii. $\overline{M_2}(B) = (D_rD_s)\big(CoM(B;r,s)\big)|_{r=s=1} = 1170$
iii. $\overline{MM_2}(B) = (S_rS_s)\big(CoM(B;r,s)\big)|_{r=s=1} = 48.5972$
iv. $\overline{ReZ}(B) = (D_rD_s)(D_r + D_s)\big(CoM(B;r,s)\big)|_{r=s=1} = 5842$
v. $\overline{SDD}(B) = (D_rS_s + D_sS_r)\big(CoM(B;r,s)\big)|_{r=s=1} = 549.5$
vi. $\overline{H}(B) = 2S_rJ\big(CoM(B;r,s)\big)|_{r=s=1} = 288.8$
vii. $\overline{I}(B) = S_rJ(D_rD_s)\big(CoM(B;r,s)\big)|_{r=s=1} = 239.95$
viii. $\overline{F}(B) = (D_r^2 + D_s^2)\ \big(CoM(B;r,s)\big)|_{r=s=1} = 2728$

Hence, the proof.

Theorem 3.3. The CoM – polynomial of the molecular graph of the drug Dutasteride (C) is

$$CoM(C;r,s) = 98r^1s^3 + 32r^1s^4 + 73r^2s^2 + 116r^2s^3 + 50r^2s^4 + 41r^3s^3 + 34r^3s^4.$$

Proof:

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Let C be the molecular graph of the drug Dutasteride with $|V(C)| = 37$ and $|E(C)| = 40$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the Dutasteride molecular graph can be partitioned as illustrated in Tables 6 & 7.

TABLE .6. *Partition of vertices*

$n_i = \|V_i\|$	n_1	n_2	n_3	n_4
Number of vertices of degree i	10	13	10	4

TABLE .7. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}
Number of edges with i & j as the adjacent vertices	2	8	5	14	2	4	6

We get

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 98$$

$$\overline{m_{14}} = n_1 n_4 - m_{14} = 32$$

$$\overline{m_{22}} = \frac{n_2(n_2 - 1)}{2} - m_{22} = 73$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 116$$

$$\overline{m_{24}} = n_2 n_4 - m_{24} = 50$$

$$\overline{m_{33}} = \frac{n_3(n_3 - 1)}{2} - m_{33} = 41$$

$$\overline{m_{34}} = n_3 n_4 - m_{34} = 34$$

The CoM – polynomial of the graph C is

$$CoM(C; r, s) = \sum_{i \le j} \overline{m_{\iota J}} r^i s^j$$

$$= \overline{m_{13}} r^1 s^3 + \overline{m_{14}} r^1 s^4 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{24}} r^2 s^4 + \overline{m_{33}} r^3 s^3 + \overline{m_{34}} r^3 s^4$$

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$= 98r^1s^3 + 32r^1s^4 + 73r^2s^2 + 116r^2s^3 + 50r^2s^4 + 41r^3s^3 + 34r^3s^4.$$

Hence, the proof.

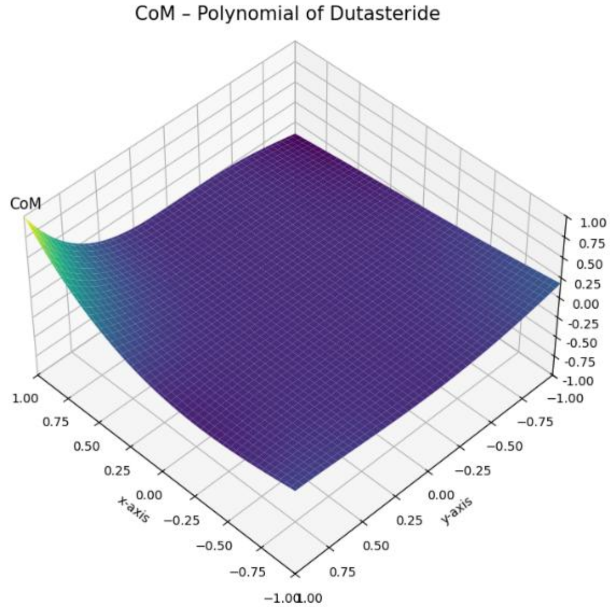


Figure 4: CoM – Polynomial of Dutasteride

Proposition: 3.3

The degree based topological coindices of C is

i. $\overline{M_1}(C) = 2208$
ii. $\overline{M_2}(C) = 2587$
iii. $\overline{MM_2}(C) = 91.8889$
iv. $\overline{ReZ}(C) = 13934$
v. $\overline{SDD}(C) = 1137.8333$
vi. $\overline{H}(C) = 92.3738$
vii. $\overline{I}(C) = 497.7524$
viii. $\overline{F}(C) = 6204$

Proof: We use $CoM(C; r, s) = 98r^1s^3 + 32r^1s^4 + 73r^2s^2 + 116r^2s^3 + 50r^2s^4 + 41r^3s^3 + 34r^3s^4$ to arrive at the following conclusions:

$$D_r = 98r^1s^3 + 32r^1s^4 + 146r^2s^2 + 232r^2s^3 + 100r^2s^4 + 123r^3s^3 + 102r^3s^4$$

$$D_s = 294r^1s^3 + 128r^1s^4 + 146r^2s^2 + 348r^2s^3 + 200r^2s^4 + 123r^3s^3 + 136r^3s^4$$

$$D_r + D_s = 392r^1s^3 + 160r^1s^4 + 292r^2s^2 + 580r^2s^3 + 300r^2s^4 + 246r^3s^3 + 238r^3s^4$$

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$D_rD_s = 294r^1s^3 + 128r^1s^4 + 292r^2s^2 + 696r^2s^3 + 400r^2s^4 + 369r^3s^3 + 408r^3s^4$$

$$D_r^2 = 98r^1s^3 + 32r^1s^4 + 292r^2s^2 + 464r^2s^3 + 200r^2s^4 + 369r^3s^3 + 306r^3s^4$$

$$D_s^2 = 882r^1s^3 + 512r^1s^4 + 292r^2s^2 + 1044r^2s^3 + 800r^2s^4 + 369r^3s^3 + 544r^3s^4$$

$$D_r^2 + D_s^2 = 980r^1s^3 + 544r^1s^4 + 584r^2s^2 + 1508r^2s^3 + 100r^2s^4 + 738r^3s^3 + 850r^3s^4$$

$$D_rD_s(D_r + D_s) = 1176r^1s^3 + 640r^1s^4 + 1168r^2s^2 + 3480r^2s^3 + 2400r^2s^4 + 2214r^3s^3 + 2856r^3s^4$$

$$S_r = 98r^1s^3 + 32r^1s^4 + \frac{73}{2}r^2s^2 + \frac{116}{2}r^2s^3 + \frac{50}{2}r^2s^4 + \frac{41}{3}r^3s^3 + \frac{34}{3}r^3s^4$$

$$S_s = \frac{98}{3}r^1s^3 + \frac{32}{4}r^1s^4 + \frac{73}{2}r^2s^2 + \frac{116}{3}r^2s^3 + \frac{50}{4}r^2s^4 + \frac{41}{3}r^3s^3 + \frac{34}{4}r^3s^4$$

$$S_rS_s = \frac{98}{3}r^1s^3 + \frac{32}{4}r^1s^4 + \frac{73}{4}r^2s^2 + \frac{116}{6}r^2s^3 + \frac{50}{8}r^2s^4 + \frac{41}{9}r^3s^3 + \frac{34}{12}r^3s^4$$

$$D_rS_s + D_sS_r = \frac{980}{3}r^1s^3 + 136r^1s^4 + 146r^2s^2 + \frac{754}{3}r^2s^3 + 125r^2s^4 + 82r^3s^3 + \frac{425}{6}r^3s^4$$

$$S_rJ = \frac{171}{4}r^4 + \frac{148}{5}r^5 + \frac{91}{6}r^6 + \frac{34}{7}r^7$$

$$S_rJ(D_rD_s) = \frac{586}{4}r^4 + \frac{824}{5}r^5 + \frac{769}{6}r^6 + \frac{408}{7}r^7$$

Thus, we get

i. $\overline{M_1}(C) = (D_r + D_s)\big(CoM(C;r,s)\big)|_{r=s=1} = 2208$
ii. $\overline{M_2}(C) = (D_rD_s)\big(CoM(C;r,s)\big)|_{r=s=1} = 2587$
iii. $\overline{MM_2}(C) = (S_rS_s)\big(CoM(C;r,s)\big)|_{r=s=1} = 91.8889$
iv. $\overline{ReZ}(C) = (D_rD_s)(D_r + D_s)\big(CoM(C;r,s)\big)|_{r=s=1} = 13934$
v. $\overline{SDD}(C) = (D_rS_s + D_sS_r)\big(CoM(C;r,s)\big)|_{r=s=1} = 1137.8333$
vi. $\overline{H}(C) = 2S_rJ\big(CoM(C;r,s)\big)|_{r=s=1} = 92.3738$
vii. $\overline{I}(C) = S_rJ(D_rD_s)\big(CoM(C;r,s)\big)|_{r=s=1} = 497.7524$
viii. $\overline{F}(C) = (D_r^2 + D_s^2)\ \big(CoM(C;r,s)\big)|_{r=s=1} = 6204$

Hence, the proof.

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Theorem 3.4. The CoM – polynomial of the molecular graph of the drug Biotin (D) is

$$CoM(D;r,s) = 12rs^3 + 24r^2s^2 + 32r^2s^3 + 8r^3s^3.$$

Proof:

Let D be the molecular graph of the drug Biotin with $|V(D)| = 16$ and $|E(D)| = 17$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the Biotin molecular graph can be partitioned as illustrated in Tables 8 & 9.

TABLE .8. *Partition of vertices*

$n_i = \lvert V_i \rvert$	n_1	n_2	n_3
Number of vertices of degree i	3	8	5

TABLE .9. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{13}	m_{22}	m_{23}	m_{33}
Number of edges with i & j as the adjacent vertices	3	4	8	2

We get

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 12$$

$$\overline{m_{22}} = \frac{n_2(n_2 - 1)}{2} - m_{22} = 24$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 32$$

$$\overline{m_{33}} = \frac{n_3(n_3 - 1)}{2} - m_{33} = 8$$

The CoM – polynomial of the graph D is

$$CoM(D;r,s) = \sum_{i \le j} \overline{m_{ij}} r^i s^j$$

Received: August 07 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$= \overline{m_{13}}r^1s^3 + \overline{m_{22}}r^2s^2 + \overline{m_{23}}r^2s^3 + \overline{m_{33}}r^3s^3$$

$$= 12r^1s^3 + 24r^2s^2 + 32r^2s^3 + 8r^3s^3.$$

Hence, the proof.

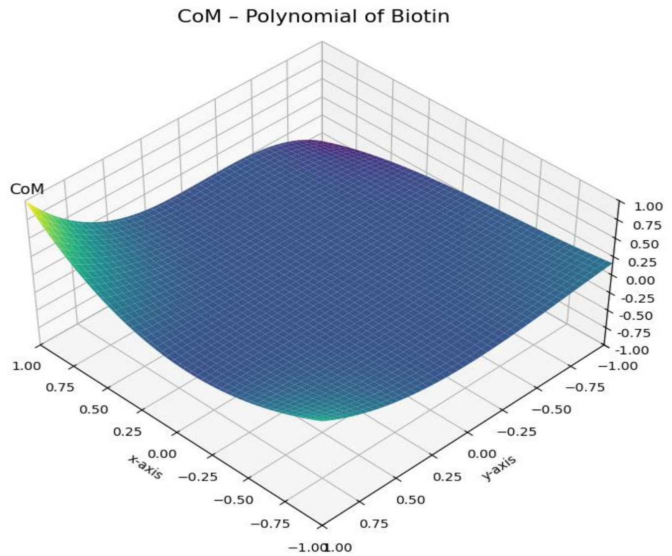


Figure 5: CoM – Polynomial of Biotin

Proposition: 3.4

The degree based topological coindices of D is

i. $\overline{M_1}(D) = 352$
ii. $\overline{M_2}(D) = 396$
iii. $\overline{MM_2}(D) = 16.2222$
iv. $\overline{ReZ}(D) = 1920$
v. $\overline{SDD}(D) = 173.3333$
vi. $\overline{H}(D) = 33.4667$
vii. $\overline{I}(D) = 83.4$
viii. $\overline{F}(D) = 872$

Proof: We use $CoM(D; r, s) = 12r^1s^3 + 24r^2s^2 + 32r^2s^3 + 8r^3s^3$ to arrive at the following conclusions:

$$D_r = 12r^1s^3 + 48r^2s^2 + 64r^2s^3 + 24r^3s^3$$

$$D_s = 36r^1s^3 + 48r^2s^2 + 96r^2s^3 + 24r^3s^3$$

Received: August 07 2025

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$D_r + D_s = 48r^1s^3 + 96r^2s^2 + 160r^2s^3 + 48r^3s^3$$

$$D_rD_s = 36r^1s^3 + 96r^2s^2 + 192r^2s^3 + 72r^3s^3$$

$$D_r^2 = 12r^1s^3 + 96r^2s^2 + 128r^2s^3 + 72r^3s^3$$

$$D_s^2 = 108r^1s^3 + 96r^2s^2 + 288r^2s^3 + 72r^3s^3$$

$$D_r^2 + D_s^2 = 120r^1s^3 + 192r^2s^2 + 416r^2s^3 + 144r^3s^3$$

$$D_rD_s(D_r + D_s) = 144r^1s^3 + 384r^2s^2 + 960r^2s^3 + 432r^3s^3$$

$$S_r = 12r^1s^3 + 12r^2s^2 + 16r^2s^3 + \frac{8}{3}r^3s^3$$

$$S_s = 4r^1s^3 + 12r^2s^2 + \frac{32}{3}r^2s^3 + \frac{8}{3}r^3s^3$$

$$S_rS_s = 4r^1s^3 + 6r^2s^2 + \frac{32}{6}r^2s^3 + \frac{8}{9}r^3s^3$$

$$D_rS_s + D_sS_r = 40r^1s^3 + 48r^2s^2 + \frac{208}{3}r^2s^3 + 16r^3s^3$$

$$S_rJ = 9r^4 + \frac{32}{5}r^5 + \frac{8}{6}r^6$$

$$S_rJ(D_rD_s) = \frac{132}{4}r^4 + \frac{192}{5}r^5 + \frac{72}{6}r^6$$

Thus, we get

i. $\overline{M_1}(D) = (D_r + D_s)\big(CoM(D;r,s)\big)|_{r=s=1} = 352$
ii. $\overline{M_2}(D) = (D_rD_s)\big(CoM(D;r,s)\big)|_{r=s=1} = 396$
iii. $\overline{MM_2}(D) = (S_rS_s)\big(CoM(D;r,s)\big)|_{r=s=1} = 16.2222$
iv. $\overline{ReZ}(D) = (D_rD_s)(D_r + D_s)\big(CoM(D;r,s)\big)|_{r=s=1} = 1920$
v. $\overline{SDD}(D) = (D_rS_s + D_sS_r)\big(CoM(D;r,s)\big)|_{r=s=1} = 173.3333$
vi. $\overline{H}(D) = 2S_rJ\big(CoM(D;r,s)\big)|_{r=s=1} = 33.4667$
vii. $\overline{I}(D) = S_rJ(D_rD_s)\big(CoM(D;r,s)\big)|_{r=s=1} = 83.4$
viii. $\overline{F}(D) = (D_r^2 + D_s^2)\big(CoM(D;r,s)\big)|_{r=s=1} = 872$

Hence, the proof.

Theorem 3.5. The CoM – polynomial of the molecular graph of the drug Triamcinolone (F) is

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$CoM(F;r,s) = 71r^1s^2 + 59r^1s^3 + 32r^1s^4 + 26r^2s^2 + 47r^2s^3 + 30r^2s^4 + 20r^3s^3 + 22r^3s^4 + 4r^4s^4$.

Proof:

Let F be the molecular graph of the drug Triamcinolone with $|V(F)| = 28$ and $|E(F)| = 31$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the Triamcinolone molecular graph can be partitioned as illustrated in Tables 10 & 11.

TABLE .10. *Partition of vertices*

$n_i = \|V_i\|$	n_1	n_2	n_3	n_4
Number of vertices of degree i	9	8	7	4

TABLE .11. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}
Number of edges with i & j as the adjacent vertices	1	4	4	2	9	2	1	6	2

We get

$$\overline{m_{12}} = n_1n_2 - m_{12} = 71$$

$$\overline{m_{13}} = n_1n_3 - m_{13} = 59$$

$$\overline{m_{14}} = n_1n_4 - m_{14} = 32$$

$$\overline{m_{22}} = \frac{n_2(n_2-1)}{2} - m_{22} = 26$$

$$\overline{m_{23}} = n_2n_3 - m_{23} = 47$$

$$\overline{m_{24}} = n_2n_4 - m_{24} = 30$$

$$\overline{m_{33}} = \frac{n_3(n_3-1)}{2} - m_{33} = 20$$

$$\overline{m_{34}} = n_3n_4 - m_{34} = 22$$

Received: August 07 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$\overline{m_{44}} = \frac{n_4(n_4 - 1)}{2} - m_{44} = 4$$

The CoM – polynomial of the graph F is

$$CoM(F; r, s) = \sum_{i \le j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{12}} r^1 s^2 + \overline{m_{13}} r^1 s^3 + \overline{m_{14}} r^1 s^4 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{24}} r^2 s^4 + \overline{m_{33}} r^3 s^3 + \overline{m_{34}} r^3 s^4 + \overline{m_{44}} r^4 s^4$$

$$= 71r^1s^2 + 59r^1s^3 + 32r^1s^4 + 26r^2s^2 + 47r^2s^3 + 30r^2s^4 + 20r^3s^3 + 22r^3s^4 + 4r^4s^4.$$

Hence, the proof.

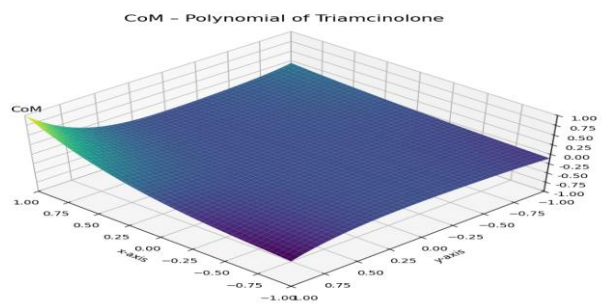


Figure 6: CoM – Polynomial of Triamcinolone

Proposition: 3.5

The degree based topological coindices of F is

i. $\overline{M_1}(F) = 1434$
ii. $\overline{M_2}(F) = 1581$
iii. $\overline{MM_2}(F) = 85.5556$
iv. $\overline{ReZ}(F) = 8480$
v. $\overline{SDD}(F) = 832.8333$
vi. $\overline{H}(F) = 145.3857$
vii. $\overline{I}(F) = 315.2976$
viii. $\overline{F}(F) = 3946$

Proof: We use $CoM(F; r, s) = 71r^1s^2 + 59r^1s^3 + 32r^1s^4 + 26r^2s^2 + 47r^2s^3 + 30r^2s^4 + 20r^3s^3 + 22r^3s^4 + 4r^4s^4$ to arrive at the following conclusions:

$$D_r = 71r^1s^2 + 59r^1s^3 + 32r^1s^4 + 52r^2s^2 + 94r^2s^3 + 60r^2s^4 + 60r^3s^3 + 66r^3s^4 + 16r^4s^4$$

$$D_s = 142r^1s^2 + 177r^1s^3 + 128r^1s^4 + 52r^2s^2 + 141r^2s^3 + 120r^2s^4 + 60r^3s^3 + 88r^3s^4 + 16r^4s^4$$

$$D_r + D_s = 213r^1s^2 + 236r^1s^3 + 160r^1s^4 + 104r^2s^2 + 235r^2s^3 + 180r^2s^4 + 120r^3s^3 + 154r^3s^4 + 32r^4s^4$$

$$D_rD_s = 142r^1s^2 + 177r^1s^3 + 128r^1s^4 + 104r^2s^2 + 282r^2s^3 + 240r^2s^4 + 180r^3s^3 + 264r^3s^4 + 64r^4s^4$$

$$D_r^2 = 71r^1s^2 + 59r^1s^3 + 32r^1s^4 + 104r^2s^2 + 188r^2s^3 + 120r^2s^4 + 180r^3s^3 + 198r^3s^4 + 64r^4s^4$$

$$D_s^2 = 284r^1s^2 + 531r^1s^3 + 512r^1s^4 + 104r^2s^2 + 423r^2s^3 + 480r^2s^4 + 180r^3s^3 + 352r^3s^4 + 64r^4s^4$$

$$D_r^2 + D_s^2 = 355r^1s^2 + 590r^1s^3 + 544r^1s^4 + 208r^2s^2 + 611r^2s^3 + 600r^2s^4 + 360r^3s^3 + 550r^3s^4 + 128r^4s^4$$

$$D_rD_s(D_r + D_s) = 426r^1s^2 + 708r^1s^3 + 640r^1s^4 + 416r^2s^2 + 1410r^2s^3 + 1440r^2s^4 + 1080r^3s^3 + 1848r^3s^4 + 512r^4s^4$$

$$S_r = 71r^1s^2 + 59r^1s^3 + 32r^1s^4 + 13r^2s^2 + \frac{47}{2}r^2s^3 + 15r^2s^4 + \frac{20}{3}r^3s^3 + \frac{22}{3}r^3s^4 + r^4s^4$$

$$S_s = \frac{71}{2}r^1s^2 + \frac{59}{3}r^1s^3 + 8r^1s^4 + 13r^2s^2 + \frac{47}{3}r^2s^3 + \frac{30}{4}r^2s^4 + \frac{20}{3}r^3s^3 + \frac{22}{4}r^3s^4 + r^4s^4$$

$$S_rS_s = \frac{71}{2}r^1s^2 + \frac{59}{3}r^1s^3 + 8r^1s^4 + \frac{13}{2}r^2s^2 + \frac{47}{6}r^2s^3 + \frac{30}{8}r^2s^4 + \frac{20}{9}r^3s^3 + \frac{22}{12}r^3s^4 + \frac{1}{4}r^4s^4$$

$$D_rS_s + D_sS_r = \frac{355}{2}r^1s^2 + \frac{590}{3}r^1s^3 + 136r^1s^4 + 52r^2s^2 + \frac{611}{6}r^2s^3 + 75r^2s^4 + 40r^3s^3 + \frac{275}{6}r^3s^4 + 8r^4s^4$$

$$S_rJ = \frac{71}{3}r^3 + \frac{85}{4}r^4 + \frac{79}{5}r^5 + \frac{50}{6}r^6 + \frac{22}{7}r^7 + \frac{1}{2}r^8$$

$$S_rJ(D_rD_s) = \frac{142}{3}r^3 + \frac{281}{4}r^4 + \frac{410}{5}r^5 + \frac{420}{6}r^6 + \frac{264}{7}r^7 + 8r^8$$

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Thus, we get

i. $\overline{M_1}(F) = (D_r + D_s)\big(CoM(F;r,s)\big)|_{r=s=1} = 1434$
ii. $\overline{M_2}(F) = (D_r D_s)\big(CoM(F;r,s)\big)|_{r=s=1} = 1581$
iii. $\overline{MM_2}(F) = (S_r S_s)\big(CoM(F;r,s)\big)|_{r=s=1} = 85.5556$
iv. $\overline{ReZ}(F) = (D_r D_s)(D_r + D_s)\big(CoM(F;r,s)\big)|_{r=s=1} = 8480$
v. $\overline{SDD}(F) = (D_r S_s + D_s S_r)\big(CoM(F;r,s)\big)|_{r=s=1} = 832.8333$
vi. $\bar{H}(F) = 2S_r J\big(CoM(F;r,s)\big)|_{r=s=1} = 145.3857$
vii. $\bar{I}(F) = S_r J(D_r D_s)\big(CoM(F;r,s)\big)|_{r=s=1} = 315.2976$
viii. $\bar{F}(F) = (D_r^2 + D_s^2)\ \big(CoM(F;r,s)\big)|_{r=s=1} = 3946$

Hence, the proof.

Theorem 3.6. The CoM – polynomial of the molecular graph of the drug Spironolactone (G) is

$$CoM(G;r,s) = 44r^1s^3 + 16r^1s^4 + 62r^2s^2 + 85r^2s^3 + 31r^2s^4 + 25r^3s^3 + 21r^3s^4 + 2r^4s^4.$$

Proof:

Let G be the molecular graph of the drug Spironolactone with $|V(G)| = 29$ and $|E(G)| = 33$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the Spironolactone molecular graph can be partitioned as illustrated in Tables 12 & 13.

TABLE .12. *Partition of vertices*

$n_i = \|V_i\|$	n_1	n_2	n_3	n_4
Number of vertices of degree i	6	12	8	3

TABLE .13. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}
Number of edges with i & j as the adjacent vertices	4	2	4	11	5	3	3	1

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

We get

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 44$$

$$\overline{m_{14}} = n_1 n_4 - m_{14} = 16$$

$$\overline{m_{22}} = \frac{n_2(n_2-1)}{2} - m_{22} = 62$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 85$$

$$\overline{m_{24}} = n_2 n_4 - m_{24} = 31$$

$$\overline{m_{33}} = \frac{n_3(n_3-1)}{2} - m_{33} = 25$$

$$\overline{m_{34}} = n_3 n_4 - m_{34} = 21$$

$$\overline{m_{44}} = \frac{n_4(n_4-1)}{2} - m_{44} = 2$$

The CoM – polynomial of the graph G is

$$CoM(G; r, s) = \sum_{i \le j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{13}} r^1 s^3 + \overline{m_{14}} r^1 s^4 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{24}} r^2 s^4 + \overline{m_{33}} r^3 s^3 + \overline{m_{34}} r^3 s^4 + \overline{m_{44}} r^4 s^4$$

$$= 44r^1 s^3 + 16r^1 s^4 + 62r^2 s^2 + 85r^2 s^3 + 31r^2 s^4 + 25r^3 s^3 + 21r^3 s^4 + 2r^4 s^4.$$

Hence, the proof.

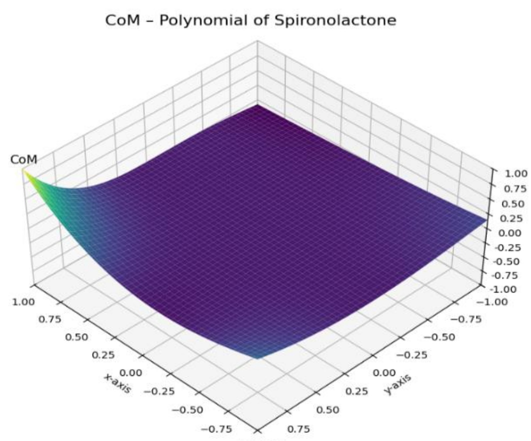


Figure 7: CoM – Polynomial of Spironolactone

Proposition: 3.6

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

The degree based topological coindices of G is

i. $\overline{M_1}(G) = 1428$
ii. $\overline{M_2}(G) = 1711$
iii. $\overline{MM_2}(G) = 56.8611$
iv. $\overline{ReZ}(G) = 9248$
v. $\overline{SDD}(G) = 698.0833$
vi. $\overline{H}(G) = 118.5667$
vii. $\overline{I}(G) = 328.6333$
viii. $\overline{F}(G) = 3972$

Proof: We use $CoM(G;r,s) = 44r^1s^3 + 16r^1s^4 + 62r^2s^2 + 85r^2s^3 + 31r^2s^4 + 25r^3s^3 + 21r^3s^4 + 2r^4s^4$ to arrive at the following conclusions:

$$D_r = 44r^1s^3 + 16r^1s^4 + 124r^2s^2 + 170r^2s^3 + 62r^2s^4 + 75r^3s^3 + 63r^3s^4 + 8r^4s^4$$

$$D_s = 132r^1s^3 + 64r^1s^4 + 124r^2s^2 + 255r^2s^3 + 124r^2s^4 + 75r^3s^3 + 84r^3s^4 + 8r^4s^4$$

$$D_r + D_s = 176r^1s^3 + 80r^1s^4 + 248r^2s^2 + 425r^2s^3 + 186r^2s^4 + 150r^3s^3 + 147r^3s^4 + 16r^4s^4$$

$$D_rD_s = 132r^1s^3 + 64r^1s^4 + 248r^2s^2 + 510r^2s^3 + 248r^2s^4 + 225r^3s^3 + 252r^3s^4 + 32r^4s^4$$

$$D_r^2 = 44r^1s^3 + 16r^1s^4 + 248r^2s^2 + 340r^2s^3 + 124r^2s^4 + 225r^3s^3 + 189r^3s^4 + 32r^4s^4$$

$$D_s^2 = 396r^1s^3 + 256r^1s^4 + 248r^2s^2 + 765r^2s^3 + 496r^2s^4 + 225r^3s^3 + 336r^3s^4 + 32r^4s^4$$

$$D_r^2 + D_s^2 = 440r^1s^3 + 272r^1s^4 + 496r^2s^2 + 1105r^2s^3 + 620r^2s^4 + 450r^3s^3 + 525r^3s^4 + 64r^4s^4$$

$$D_rD_s(D_r + D_s) = 528r^1s^3 + 320r^1s^4 + 992r^2s^2 + 2550r^2s^3 + 1488r^2s^4 + 1350r^3s^3 + 1764r^3s^4 + 256r^4s^4$$

$$S_r = 44r^1s^3 + 16r^1s^4 + 31r^2s^2 + \frac{85}{2}r^2s^3 + \frac{31}{2}r^2s^4 + \frac{25}{3}r^3s^3 + \frac{21}{3}r^3s^4 + \frac{1}{2}r^4s^4$$

$$S_s = \frac{44}{3}r^1s^3 + 4r^1s^4 + 31r^2s^2 + \frac{85}{3}r^2s^3 + \frac{31}{4}r^2s^4 + \frac{25}{3}r^3s^3 + \frac{21}{4}r^3s^4 + \frac{1}{2}r^4s^4$$

$$S_rS_s = \frac{44}{3}r^1s^3 + 4r^1s^4 + \frac{31}{2}r^2s^2 + \frac{85}{6}r^2s^3 + \frac{31}{8}r^2s^4 + \frac{25}{9}r^3s^3 + \frac{21}{12}r^3s^4 + \frac{1}{8}r^4s^4$$

Received: August 07 2025

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$D_rS_s + D_sS_r = \frac{440}{3}r^1s^3 + 68r^1s^4 + 124r^2s^2 + \frac{1105}{6}r^2s^3 + \frac{155}{2}r^2s^4 + 50r^3s^3 + \frac{175}{6}r^3s^4 + 4r^4s^4$$

$$S_rJ = \frac{106}{4}r^4 + \frac{101}{5}r^5 + \frac{56}{6}r^6 + \frac{21}{7}r^7 + \frac{1}{4}r^8$$

$$S_rJ(D_rD_s) = \frac{380}{4}r^4 + \frac{574}{5}r^5 + \frac{473}{6}r^6 + \frac{252}{7}r^7 + 4r^8$$

Thus, we get

i. $\overline{M_1}(G) = (D_r + D_s)\big(CoM(G;r,s)\big)|_{r=s=1} = 1428$
ii. $\overline{M_2}(G) = (D_rD_s)\big(CoM(G;r,s)\big)|_{r=s=1} = 1711$
iii. $\overline{MM_2}(G) = (S_rS_s)\big(CoM(G;r,s)\big)|_{r=s=1} = 56.8611$
iv. $\overline{ReZ}(G) = (D_rD_s)(D_r + D_s)\big(CoM(G;r,s)\big)|_{r=s=1} = 9248$
v. $\overline{SDD}(G) = (D_rS_s + D_sS_r)\big(CoM(G;r,s)\big)|_{r=s=1} = 698.0833$
vi. $\overline{H}(G) = 2S_rJ\big(CoM(G;r,s)\big)|_{r=s=1} = 118.5667$
vii. $\overline{I}(G) = S_rJ(D_rD_s)\big(CoM(G;r,s)\big)|_{r=s=1} = 328.6333$
viii. $\overline{F}(G) = (D_r^2 + D_s^2)\,\big(CoM(G;r,s)\big)|_{r=s=1} = 3972$

Hence, the proof.

Theorem 3.7. The CoM – polynomial of the molecular graph of the drug Ritlecitinib (H) is

$$CoM(H;r,s) = 32rs^2 + 19rs^3 + 50r^2s^2 + 66r^2s^3 + 17r^3s^3.$$

Proof:

Let H be the molecular graph of the drug Ritlecitinib with $|V(H)| = 21$ and $|E(H)| = 23$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i,j. The vertices and edges of the Ritlecitinib molecular graph can be partitioned as illustrated in Tables 14 & 15.

TABLE .14. *Partition of vertices*

$n_i = \lvert V_i\rvert$	n_1	n_2	n_3
Number of vertices of degree i	3	11	7

International Journal of Applied Mathematics

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

TABLE .15. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{12}	m_{13}	m_{22}	m_{23}	m_{33}
Number of edges with i & j as the adjacent vertices	1	2	5	11	4

We get

$$\overline{m_{12}} = n_1 n_2 - m_{12} = 32$$

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 19$$

$$\overline{m_{22}} = \frac{n_2(n_2 - 1)}{2} - m_{22} = 50$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 66$$

$$\overline{m_{33}} = \frac{n_3(n_3 - 1)}{2} - m_{33} = 17$$

The CoM – polynomial of the graph H is

$$CoM(H; r, s) = \sum_{i \le j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{12}} r^1 s^2 + \overline{m_{13}} r^1 s^3 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{33}} r^3 s^3$$

$$= 32r^1 s^2 + 19r^1 s^3 + 50r^2 s^2 + 66r^2 s^3 + 17r^3 s^3.$$

Hence, the proof.

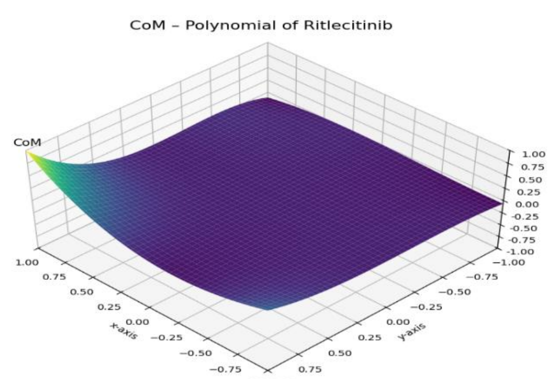


Figure 8: CoM – Polynomial of Ritlecitinib

Received: August 07 2025

International Journal of Applied Mathematics

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Proposition: 3.7

The degree based topological coindices of H is

i. $\overline{M_1}(H) = 804$
ii. $\overline{M_2}(H) = 870$
iii. $\overline{MM_2}(H) = 47.7222$
iv. $\overline{ReZ}(H) = 4118$
v. $\overline{SDD}(H) = 420.3333$
vi. $\overline{H}(H) = 87.9$
vii. $\overline{I}(H) = 190.2833$
viii. $\overline{F}(H) = 1914$

Proof: We use $CoM(H;r,s) = 32r^1s^2 + 19r^1s^3 + 50r^2s^2 + 66r^2s^3 + 17r^3s^3$ to arrive at the following conclusions:

$$D_r = 32r^1s^2 + 19r^1s^3 + 100r^2s^2 + 132r^2s^3 + 51r^3s^3$$

$$D_s = 64r^1s^2 + 57r^1s^3 + 100r^2s^2 + 198r^2s^3 + 51r^3s^3$$

$$D_r + D_s = 96r^1s^2 + 76r^1s^3 + 200r^2s^2 + 330r^2s^3 + 102r^3s^3$$

$$D_rD_s = 64r^1s^2 + 57r^1s^3 + 200r^2s^2 + 396r^2s^3 + 153r^3s^3$$

$$D_r^2 = 32r^1s^2 + 19r^1s^3 + 200r^2s^2 + 264r^2s^3 + 153r^3s^3$$

$$D_s^2 = 128r^1s^2 + 171r^1s^3 + 200r^2s^2 + 594r^2s^3 + 153r^3s^3$$

$$D_r^2 + D_s^2 = 160r^1s^2 + 190r^1s^3 + 400r^2s^2 + 858r^2s^3 + 306r^3s^3$$

$$D_rD_s(D_r + D_s) = 192r^1s^2 + 228r^1s^3 + 800r^2s^2 + 1980r^2s^3 + 918r^3s^3$$

$$S_r = 32r^1s^2 + 19r^1s^3 + 25r^2s^2 + 33r^2s^3 + \frac{17}{3}r^3s^3$$

$$S_s = 16r^1s^2 + \frac{19}{3}r^1s^3 + 25r^2s^2 + 22r^2s^3 + \frac{17}{3}r^3s^3$$

$$S_rS_s = 16r^1s^2 + \frac{19}{3}r^1s^3 + \frac{25}{2}r^2s^2 + 11r^2s^3 + \frac{17}{9}r^3s^3$$

$$D_rS_s + D_sS_r = 80r^1s^2 + \frac{190}{3}r^1s^3 + 100r^2s^2 + 143r^2s^3 + 34r^3s^3$$

$$S_rJ = \frac{32}{3}r^3 + \frac{69}{4}r^4 + \frac{66}{5}r^5 + \frac{17}{6}r^6$$

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$S_rJ(D_rD_s) = \frac{64}{3}r^3 + \frac{257}{4}r^4 + \frac{396}{5}r^5 + \frac{153}{6}r^6$$

Thus, we get

i. $\overline{M_1}(H) = (D_r + D_s)\big(CoM(H;r,s)\big)|_{r=s=1} = 804$
ii. $\overline{M_2}(H) = (D_rD_s)\big(CoM(H;r,s)\big)|_{r=s=1} = 870$
iii. $\overline{MM_2}(H) = (S_rS_s)\big(CoM(H;r,s)\big)|_{r=s=1} = 47.7222$
iv. $\overline{ReZ}(H) = (D_rD_s)(D_r + D_s)\big(CoM(H;r,s)\big)|_{r=s=1} = 4118$
v. $\overline{SDD}(H) = (D_rS_s + D_sS_r)\big(CoM(H;r,s)\big)|_{r=s=1} = 420.3333$
vi. $\overline{H}(H) = 2S_rJ\big(CoM(H;r,s)\big)|_{r=s=1} = 87.9$
vii. $\overline{I}(H) = S_rJ(D_rD_s)\big(CoM(H;r,s)\big)|_{r=s=1} = 190.2833$
viii. $\overline{F}(H) = (D_r^2 + D_s^2)\ \big(CoM(H;r,s)\big)|_{r=s=1} = 1914$

Hence, the proof.

Theorem 3.8. The CoM – polynomial of the molecular graph of the drug Baricitinib (I) is

$$CoM(I;r,s) = 54r^1s^2 + 6r^1s^4 + 85r^2s^2 + 74r^2s^3 + 24r^2s^4 + 12r^3s^3 + 10r^3s^4.$$

Proof:

Let I be the molecular graph of the drug Baricitinib with $|V(I)| = 26$ and $|E(I)| = 29$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i,j. The vertices and edges of the Baricitinib molecular graph can be partitioned as illustrated in Tables 16 & 17.

TABLE .16. *Partition of vertices*

$n_i = \lvert V_i \rvert$	n_1	n_2	n_3	n_4
Number of vertices of degree i	4	14	6	2

TABLE .17. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{12}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}
Number of edges with	2	2	6	10	4	3	2

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

i & j as the adjacent vertices							

We get

$$\overline{m_{12}} = n_1 n_2 - m_{12} = 54$$

$$\overline{m_{14}} = n_1 n_4 - m_{14} = 6$$

$$\overline{m_{22}} = \frac{n_2(n_2-1)}{2} - m_{22} = 85$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 74$$

$$\overline{m_{24}} = n_2 n_4 - m_{24} = 24$$

$$\overline{m_{33}} = \frac{n_3(n_3-1)}{2} - m_{33} = 12$$

$$\overline{m_{34}} = n_3 n_4 - m_{34} = 10$$

The CoM – polynomial of the graph I is

$$CoM(I; r, s) = \sum_{i \le j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{12}} r^1 s^2 + \overline{m_{14}} r^1 s^4 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{24}} r^2 s^4 + \overline{m_{33}} r^3 s^3 + \overline{m_{34}} r^3 s^4$$

$$= 54 r^1 s^2 + 6 r^1 s^4 + 85 r^2 s^2 + 74 r^2 s^3 + 24 r^2 s^4 + 12 r^3 s^3 + 10 r^3 s^4.$$

Hence, the proof.

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

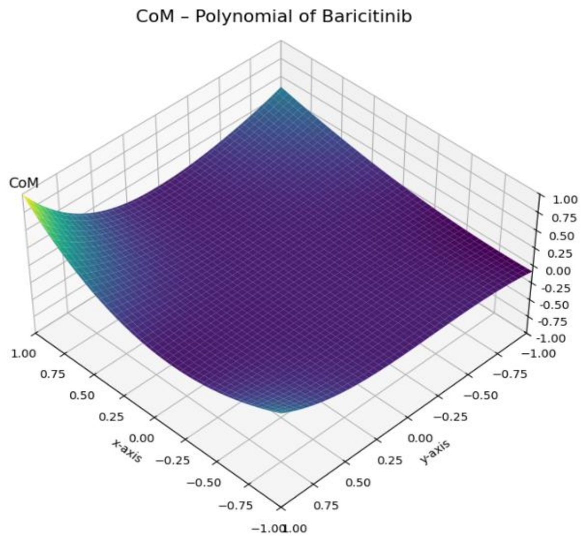


Figure 9: CoM – Polynomial of Baricitinib

Proposition: 3.8

The degree based topological coindices of I is

i. $\overline{M_1}(I) = 1188$
ii. $\overline{M_2}(I) = 1336$
iii. $\overline{MM_2}(I) = 67.25$
iv. $\overline{ReZ}(I) = 6664$
v. $\overline{SDD}(I) = 595.6667$
vi. $\overline{H}(I) = 125.3571$
vii. $\overline{I}(I) = 281.7429$
viii. $\overline{F}(I) = 2960$

Proof: We use $CoM(I;r,s) = 54r^1s^2 + 6r^1s^4 + 85r^2s^2 + 74r^2s^3 + 24r^2s^4 + 12r^3s^3 + 10r^3s^4$ to arrive at the following conclusions:

$$D_r = 54r^1s^2 + 6r^1s^4 + 170r^2s^2 + 148r^2s^3 + 48r^2s^4 + 36r^3s^3 + 30r^3s^4$$

$$D_s = 108r^1s^2 + 24r^1s^4 + 170r^2s^2 + 222r^2s^3 + 96r^2s^4 + 36r^3s^3 + 40r^3s^4$$

$$D_r + D_s = 162r^1s^2 + 30r^1s^4 + 340r^2s^2 + 370r^2s^3 + 144r^2s^4 + 72r^3s^3 + 70r^3s^4$$

$$D_rD_s = 108r^1s^2 + 24r^1s^4 + 340r^2s^2 + 444r^2s^3 + 192r^2s^4 + 108r^3s^3 + 120r^3s^4$$

$$D_r^2 = 54r^1s^2 + 6r^1s^4 + 340r^2s^2 + 296r^2s^3 + 96r^2s^4 + 108r^3s^3 + 90r^3s^4$$

$$D_s^2 = 216r^1s^2 + 96r^1s^4 + 340r^2s^2 + 666r^2s^3 + 384r^2s^4 + 108r^3s^3 + 160r^3s^4$$

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$D_r^2 + D_s^2 = 270r^1s^2 + 102r^1s^4 + 680r^2s^2 + 962r^2s^3 + 480r^2s^4 + 216r^3s^3 + 250r^3s^4$$

$$D_rD_s(D_r + D_s) = 324r^1s^2 + 120r^1s^4 + 1360r^2s^2 + 2220r^2s^3 + 1152r^2s^4 + 648r^3s^3 + 840r^3s^4$$

$$S_r = 54r^1s^2 + 6r^1s^4 + \frac{85}{2}r^2s^2 + 37r^2s^3 + 12r^2s^4 + 4r^3s^3 + \frac{10}{3}r^3s^4$$

$$S_s = 27r^1s^2 + \frac{3}{2}r^1s^4 + \frac{85}{2}r^2s^2 + \frac{74}{3}r^2s^3 + 6r^2s^4 + 4r^3s^3 + \frac{5}{2}r^3s^4$$

$$S_rS_s = 27r^1s^2 + \frac{3}{2}r^1s^4 + \frac{85}{4}r^2s^2 + \frac{74}{6}r^2s^3 + 3r^2s^4 + \frac{4}{3}r^3s^3 + \frac{5}{6}r^3s^4$$

$$D_rS_s + D_sS_r = 135r^1s^2 + \frac{51}{2}r^1s^4 + 170r^2s^2 + \frac{481}{3}r^2s^3 + 60r^2s^4 + 24r^3s^3 + \frac{125}{6}r^3s^4$$

$$S_rJ = 36r^3 + 85r^4 + \frac{468}{5}r^5 + 50r^6 + \frac{120}{7}r^7$$

$$S_rJ(D_rD_s) = 18r^3 + \frac{85}{4}r^4 + 16r^5 + 6r^6 + \frac{10}{7}r^7$$

Thus, we get

i. $\overline{M_1}(I) = (D_r + D_s)\big(CoM(I;r,s)\big)|_{r=s=1} = 1188$
ii. $\overline{M_2}(I) = (D_rD_s)\big(CoM(I;r,s)\big)|_{r=s=1} = 1336$
iii. $\overline{MM_2}(I) = (S_rS_s)\big(CoM(I;r,s)\big)|_{r=s=1} = 67.25$
iv. $\overline{ReZ}(I) = (D_rD_s)(D_r + D_s)\big(CoM(I;r,s)\big)|_{r=s=1} = 6664$
v. $\overline{SDD}(I) = (D_rS_s + D_sS_r)\big(CoM(I;r,s)\big)|_{r=s=1} = 595.6667$
vi. $\overline{H}(I) = 2S_rJ\big(CoM(I;r,s)\big)|_{r=s=1} = 125.3571$
vii. $\overline{I}(I) = S_rJ(D_rD_s)\big(CoM(I;r,s)\big)|_{r=s=1} = 281.7429$
viii. $\overline{F}(I) = (D_r^2 + D_s^2)\,\big(CoM(I;r,s)\big)|_{r=s=1} = 2960$

Hence, the proof.

Theorem 3.9. The CoM – polynomial of the molecular graph of the drug Dithranol (J) is

$$CoM(J;r,s) = 18rs^3 + 17r^2s^2 + 43r^2s^3 + 15r^3s^3.$$

Proof:

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

Let J be the molecular graph of the drug Dithranol with $|V(J)| = 17$ and $|E(A)| = 19$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and the degree of their terminal vertices i, j. The vertices and edges of the Dithranol molecular graph can be partitioned as illustrated in Tables 18 & 19.

TABLE .18. *Partition of vertices*

$n_i = \|V_i\|$	n_1	n_2	n_3
Number of vertices of degree i	3	7	7

TABLE .19. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{13}	m_{22}	m_{23}	m_{33}
Number of edges with i & j as the adjacent vertices	3	4	6	6

We get

$$\overline{m_{13}} = n_1 n_3 - m_{13} = 18$$

$$\overline{m_{22}} = \frac{n_2(n_2 - 1)}{2} - m_{22} = 17$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 43$$

$$\overline{m_{33}} = \frac{n_3(n_3 - 1)}{2} - m_{33} = 15$$

The CoM – polynomial of the graph J is

$$CoM(J; r, s) = \sum_{i \le j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{13}} r^1 s^3 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{33}} r^3 s^3$$

$$= 18r^1 s^3 + 17r^2 s^2 + 43r^2 s^3 + 15r^3 s^3.$$

Hence, the proof.

International Journal of Applied Mathematics
Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

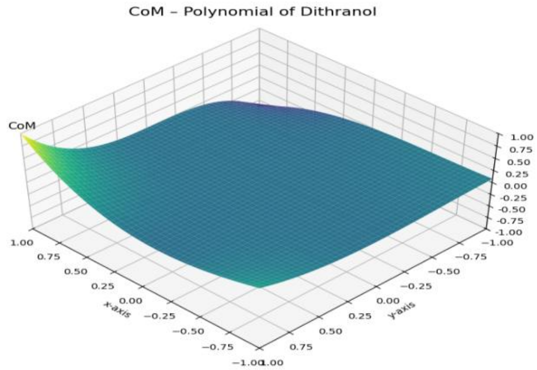


Figure 10: CoM – Polynomial of Dithranol

Proposition: 3.9

The degree based topological coindices of J is

i. $\overline{M_1}(J) = 445$
ii. $\overline{M_2}(J) = 515$
iii. $\overline{MM_2}(J) = 19.0833$
iv. $\overline{ReZ}(J) = 2588$
v. $\overline{SDD}(J) = 217.1667$
vi. $\overline{H}(J) = 39.7$
vii. $\overline{I}(J) = 104.6$
viii. $\overline{F}(J) = 1145$

Proof: We use $CoM(J; r, s) = 18r^1s^3 + 17r^2s^2 + 43r^2s^3 + 15r^3s^3$ to arrive at the following conclusions:

$$D_r = 18r^1s^3 + 34r^2s^2 + 86r^2s^3 + 45r^3s^3$$

$$D_s = 54r^1s^3 + 34r^2s^2 + 129r^2s^3 + 45r^3s^3$$

$$D_r + D_s = 72r^1s^3 + 68r^2s^2 + 215r^2s^3 + 90r^3s^3$$

$$D_rD_s = 54r^1s^3 + 68r^2s^2 + 258r^2s^3 + 135r^3s^3$$

$$D_r^2 = 18r^1s^3 + 68r^2s^2 + 172r^2s^3 + 135r^3s^3$$

$$D_s^2 = 162r^1s^3 + 68r^2s^2 + 387r^2s^3 + 135r^3s^3$$

$$D_r^2 + D_s^2 = 180r^1s^3 + 136r^2s^2 + 559r^2s^3 + 270r^3s^3$$

$$D_rD_s(D_r + D_s) = 216r^1s^3 + 272r^2s^2 + 1290r^2s^3 + 810r^3s^3$$

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$S_r = 18r^1s^3 + \frac{17}{2}r^2s^2 + \frac{43}{2}r^2s^3 + 5r^3s^3$$

$$S_s = 6r^1s^3 + \frac{17}{2}r^2s^2 + \frac{43}{3}r^2s^3 + 5r^3s^3$$

$$S_rS_s = 6r^1s^3 + \frac{17}{4}r^2s^2 + \frac{43}{6}r^2s^3 + \frac{5}{3}r^3s^3$$

$$D_rS_s + D_sS_r = 60r^1s^3 + 34r^2s^2 + \frac{559}{6}r^2s^3 + 30r^3s^3$$

$$S_rJ = \frac{35}{4}r^4 + \frac{43}{5}r^5 + \frac{15}{6}r^6$$

$$S_rJ(D_rD_s) = \frac{122}{4}r^4 + \frac{258}{5}r^5 + \frac{135}{6}r^6$$

Thus, we get

i. $\overline{M_1}(J) = (D_r + D_s)\big(CoM(J;r,s)\big)|_{r=s=1} = 445$
ii. $\overline{M_2}(J) = (D_rD_s)\big(CoM(J;r,s)\big)|_{r=s=1} = 515$
iii. $\overline{MM_2}(J) = (S_rS_s)\big(CoM(J;r,s)\big)|_{r=s=1} = 19.0833$
iv. $\overline{ReZ}(J) = (D_rD_s)(D_r + D_s)\big(CoM(J;r,s)\big)|_{r=s=1} = 2588$
v. $\overline{SDD}(J) = (D_rS_s + D_sS_r)\big(CoM(J;r,s)\big)|_{r=s=1} = 217.1667$
vi. $\overline{H}(J) = 2S_rJ\big(CoM(J;r,s)\big)|_{r=s=1} = 39.7$
vii. $\overline{I}(J) = S_rJ(D_rD_s)\big(CoM(J;r,s)\big)|_{r=s=1} = 104.6$
viii. $\overline{F}(J) = (D_r^2 + D_s^2)\ \big(CoM(J;r,s)\big)|_{r=s=1} = 1145$

Hence, the proof.

Theorem 3.10. The CoM – polynomial of the molecular graph of the drug Sulfasalazine (K) is

$$CoM(K;r,s) = 32r^1s^3 + 3r^1s^4 + 97r^2s^2 + 92r^2s^3 + 14r^2s^4 + 19r^3s^3 + 6r^3s^4.$$

Proof:

Let K be the molecular graph of the drug Sulfasalazine with $|V(K)| = 28$ and $|E(K)| = 30$. Let V_i & $E_{(i,j)}$ constitute the collection of all vertices and edges characterized by the degree of i and

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

the degree of their terminal vertices i, j. The vertices and edges of the Sulfasalazine molecular graph can be partitioned as illustrated in Tables 20 & 21.

TABLE .20. *Partition of vertices*

$n_i = \|V_i\|$	n_1	n_2	n_3	n_4
Number of vertices of degree i	5	15	7	1

TABLE .21. *Partition of edges*

$E_{(i,j)} = m_{ij}$	m_{12}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}
Number of edges with i & j as the adjacent vertices	3	2	8	13	1	2	1

We get

$$\overline{m_{13}} = n_1 n_2 - m_{12} = 32$$

$$\overline{m_{14}} = n_1 n_4 - m_{14} = 3$$

$$\overline{m_{22}} = \frac{n_2(n_2 - 1)}{2} - m_{22} = 97$$

$$\overline{m_{23}} = n_2 n_3 - m_{23} = 92$$

$$\overline{m_{24}} = n_2 n_4 - m_{24} = 14$$

$$\overline{m_{33}} = \frac{n_3(n_3 - 1)}{2} - m_{33} = 19$$

$$\overline{m_{34}} = n_3 n_4 - m_{34} = 6$$

The CoM – polynomial of the graph K is

$$CoM(K; r, s) = \sum_{i \leq j} \overline{m_{ij}} r^i s^j$$

$$= \overline{m_{13}} r^1 s^2 + \overline{m_{14}} r^1 s^4 + \overline{m_{22}} r^2 s^2 + \overline{m_{23}} r^2 s^3 + \overline{m_{24}} r^2 s^4 + \overline{m_{33}} r^3 s^3 + \overline{m_{34}} r^3 s^4$$

$$= 32 r^1 s^3 + 3 r^1 s^4 + 97 r^2 s^2 + 92 r^2 s^3 + 14 r^2 s^4 + 19 r^3 s^3 + 6 r^3 s^4.$$

Hence, the proof.

International Journal of Applied Mathematics

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

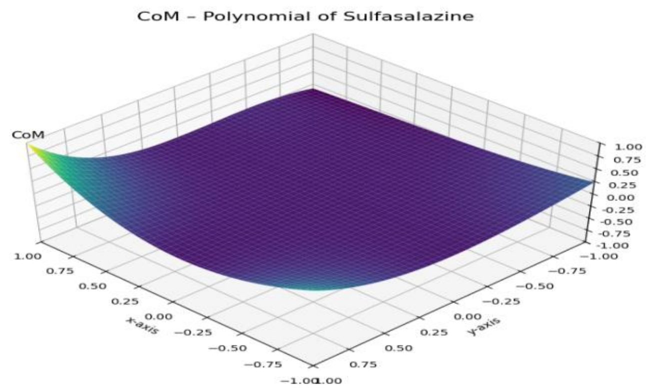


Figure 11: CoM – Polynomial of Sulfasalazine

Proposition: 3.10

The degree based topological coindices of K is

i. $\overline{M_1}(K) = 1231$
ii. $\overline{M_2}(K) = 1403$
iii. $\overline{MM_2}(K) = 55.3611$
iv. $\overline{ReZ}(K) = 6958$
v. $\overline{SDD}(K) = 598.25$
vi. $\overline{H}(K) = 115.2143$
vii. $\overline{I}(K) = 291.2524$
viii. $\overline{F}(K) = 3115$

Proof: We use $CoM(K; r, s) = 32r^1s^3 + 3r^1s^4 + 97r^2s^2 + 92r^2s^3 + 14r^2s^4 + 19r^3s^3 + 6r^3s^4$ to arrive at the following conclusions:

$$D_r = 32r^1s^3 + 3r^1s^4 + 194r^2s^2 + 184r^2s^3 + 28r^2s^4 + 57r^3s^3 + 18r^3s^4$$

$$D_s = 96r^1s^3 + 12r^1s^4 + 194r^2s^2 + 276r^2s^3 + 56r^2s^4 + 57r^3s^3 + 24r^3s^4$$

$$D_r + D_s = 128r^1s^3 + 15r^1s^4 + 388r^2s^2 + 460r^2s^3 + 84r^2s^4 + 114r^3s^3 + 42r^3s^4$$

$$D_rD_s = 96r^1s^3 + 12r^1s^4 + 388r^2s^2 + 552r^2s^3 + 112r^2s^4 + 171r^3s^3 + 72r^3s^4$$

$$D_r^2 = 32r^1s^3 + 3r^1s^4 + 388r^2s^2 + 368r^2s^3 + 56r^2s^4 + 171r^3s^3 + 54r^3s^4$$

$$D_s^2 = 288r^1s^3 + 48r^1s^4 + 388r^2s^2 + 828r^2s^3 + 224r^2s^4 + 171r^3s^3 + 96r^3s^4$$

$$D_r^2 + D_s^2 = 320r^1s^3 + 51r^1s^4 + 776r^2s^2 + 1196r^2s^3 + 280r^2s^4 + 342r^3s^3 + 150r^3s^4$$

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

$$D_rD_s(D_r+D_s) = 384r^1s^3 + 60r^1s^4 + 1552r^2s^2 + 2760r^2s^3 + 672r^2s^4 + 1026r^3s^3 + 504r^3s^4$$

$$S_r = 32r^1s^3 + 3r^1s^4 + \frac{97}{2}r^2s^2 + 46r^2s^3 + 7r^2s^4 + \frac{19}{3}r^3s^3 + 2r^3s^4$$

$$S_s = \frac{32}{3}r^1s^3 + \frac{3}{4}r^1s^4 + \frac{97}{2}r^2s^2 + \frac{92}{3}r^2s^3 + \frac{7}{2}r^2s^4 + \frac{19}{3}r^3s^3 + \frac{3}{2}r^3s^4$$

$$S_rS_s = \frac{32}{3}r^1s^3 + \frac{3}{4}r^1s^4 + \frac{97}{4}r^2s^2 + \frac{92}{6}r^2s^3 + \frac{7}{4}r^2s^4 + \frac{19}{9}r^3s^3 + \frac{1}{2}r^3s^4$$

$$D_rS_s + D_sS_r = \frac{320}{3}r^1s^2 + \frac{51}{4}r^1s^4 + 194r^2s^2 + \frac{598}{3}r^2s^3 + 35r^2s^4 + 38r^3s^3 + \frac{25}{2}r^3s^4$$

$$S_rJ = \frac{129}{4}r^4 + \frac{95}{5}r^5 + \frac{33}{6}r^6 + \frac{6}{7}r^7$$

$$S_rJ(D_rD_s) = 121r^4 + \frac{564}{5}r^5 + \frac{283}{6}r^6 + \frac{72}{7}r^7$$

Thus, we get

i. $\overline{M_1}(K) = (D_r + D_s)\big(CoM(K;r,s)\big)|_{r=s=1} = 1231$
ii. $\overline{M_2}(K) = (D_rD_s)\big(CoM(K;r,s)\big)|_{r=s=1} = 1403$
iii. $\overline{MM_2}(K) = (S_rS_s)\big(CoM(K;r,s)\big)|_{r=s=1} = 55.3611$
iv. $\overline{ReZ}(K) = (D_rD_s)(D_r + D_s)\big(CoM(K;r,s)\big)|_{r=s=1} = 6958$
v. $\overline{SDD}(K) = (D_rS_s + D_sS_r)\big(CoM(K;r,s)\big)|_{r=s=1} = 598.25$
vi. $\overline{H}(K) = 2S_rJ\big(CoM(K;r,s)\big)|_{r=s=1} = 115.2143$
vii. $\overline{I}(K) = S_rJ(D_rD_s)\big(CoM(K;r,s)\big)|_{r=s=1} = 291.2524$
viii. $\overline{F}(K) = (D_r^2 + D_s^2)\,\big(CoM(K;r,s)\big)|_{r=s=1} = 3115$

Hence, the proof.

Volume 38 No. 9s, 2025

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

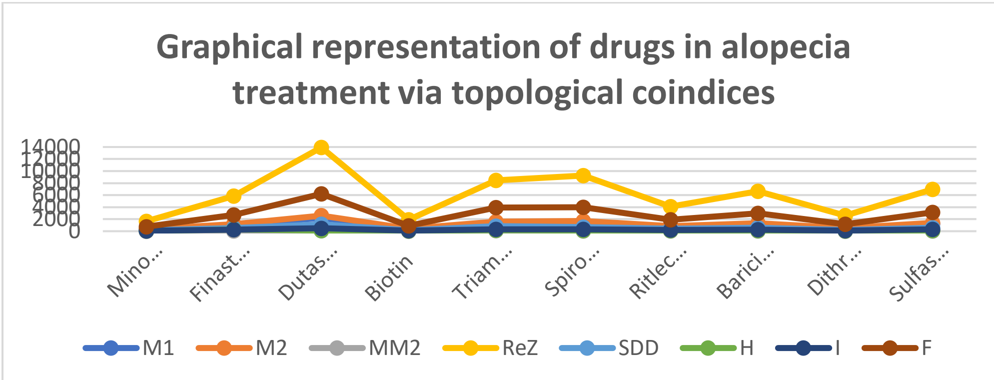


Figure 12: Graphical representation of drugs used in alopecia treatment via topological coindices

4. CONCLUSION

This work investigates the CoM-polynomial equation for the medications Minoxidil, Finasteride, Dutasteride, Biotin, Triamcinolone, Spironolactone, Ritlecitinib, Baricitinib, Dithranol and Sulfasalazine used in the treatment of alopecia. We also computed eight degree-based topological coindices for these ten medications with CoM polynomial. This work investigates using topological coindices the physicochemical characteristics of pharmaceuticals employed in alopecia therapy. Topological descriptors for drugs in the treatment of alopecia are explored in this paper together with their graphical representation in anticipating physical, chemical, and biological aspects. This paper aims to provide a comprehensive overview of current medications and their therapeutic applications, along with suggestions for future utilization. In future research, a thorough comparison of the suggested CoM polynomial model with existing computational methods and published results will be carried out. This will help us figure out how well it works, make sure it's reliable, and find ways to improve alopecia drug modeling.

REFERENCES

1. Alopecia Areata, National Institute of Arthritis and Musculoskeletal and Skin Diseases, www.nih.gov.
2. Alopecia areata available treatment, National Alopecia Areata Foundation, www.naaf.org.
3. Medications for Alopecia, Drugs used to treat Alopecia, www.drugs.com.
4. Harary F, Graph theory *Philipines: Addision – Wesley Publishing Company*, 1969.

Volume 38 No. 9s, 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

5. Trinajstic N, Chemical graph theory, *CRC Press,* Boca Raton, FL, 1993.
6. Todeschini R and Consonni V, Handbook of molecular descriptors, *Wiley Online Library,* Weinheim, 2000.
7. Hosoya H, On some counting polynomials in chemistry, *Discrete Appl. Math.,* 1988, 19, 239‑257.
8. E. Deutsch and S. Klavzar. M-polynomial and degree-based topological indices, *Iranian Journal of Mathematical Chemistry,* 2015, 6(2):93‑102.
9. Sourav Mondal, Nilanjan De, Anita Pal, On some general neighborhood degree based topological indices, *International Journal of Applied Mathematics*, 2019, vol. 32, no. 6, 1037.
10. Syed Ajaz K Kirmani, Parvez Ali, CoM-polynomial and topological coindices of hyaluronic acid conjugates, *Arabian Journal of Chemistry,* 2022, 15, 103911.
11. Akar H Karim, Nabeel E Arif, M-polynomial and CoM-polynomial of Hat-graphs, *Basrah Journal of Sciences*, 2025, 43(1), 1 – 17.
12. S. Shenbaga Devi, S. Dhanalakshmi, Computing Zagreb indices for Propranolol, *Journal of Advanced Zoology,* 2023, S8, 44.
13. S. Shenbaga Devi, S. Dhanalakshmi, Analysis of Degree-Based Topological Indices for Stroke Treatment Drugs: A Study on the Physicochemical Features, *IAENG International Journal of Applied Mathematics,* 2024, 54(6), 1233 – 1239.
14. Gutman, I. & Trinajstić, N. Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* 1972, **17**(4), 535–538.
15. S. Nikolic, G. Kovacevic, A. Milicevic, and N. Trinajstic. The zagrab indices 30 years after. *Croa. Chem. Acta*, 76(2):113‑124, 2003.
16. P.S. Ranjini, V. Lokesha, A. Usha, Relation between phenylene and hexagonal squeeze using harmonic index, *Int. J.Graph Theory*, 1, 2013, 116–121.
17. C. Gupta, V. Lokesha, S. B. Shwetha, and P. Ranjini, On the symmetric division deg index of graph, *Southeast Asian Bulletin of Mathematics*, 2016, 40(1).

18. B.S. Shetty, V. Lokesha, P.S. Ranjini, On the harmonic index of graph operations, Trans. Comb. 4 (2015), 5–14.

19. D. Vukicevic and A. Graovac. Valence connectivity versus randic, zagrab and modified zagrab index: a linear algorithm to check discriminative properties of indices in acyclic molecular graphs. Croatica Chemica Acta, 77(3):501‑508, 2004.

20. B. Furtula, I. Gutman, A forgotten topological index, J. Math. Chem. 53 (2015), 1184–1190.

21. M. C. Shanmukha, A. Usha, K. C. Shilpa, N. S. Basavarajappa, M-polynomial and neighborhood M-polynomial methods for topological indices of porous graphene, *Eur. Phys. J. Plus*, 2021, 136, 1089.

22. M. C. Shanmukha, Sokjoon Lee, A. Usha, K. C. Shilpa, Muhammad Azeem, Structural descriptors of anthracene using topological coindices through CoM-polynomial, *Journal of Intelligent & Fuzzy Systems: Applications in Engineering and Technology,* 2023, Volume 44, Issue 5.

23. Akar H. Karim, Nabeel E. Arif, M - polynomial and CoM - polynomial of Hat-graphs, *Basrah Journal of Science,* 2025, Volume 43 (1).