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Topological Indices of Certain Antiviral Drug Compound Involved In Different Eras of Hair Colouring Dye

P. Parameswari [1], S. Meenakshi[2]

[1]Research Scholar, Department of Mathematics, Vels Institute of Science Technology and Advanced Studies, Chennai, Tamilnadu.
E-mail : yall.paramu@gmail.com
[2]Associate Professor, Department of Mathematics, Vels Institute of Science Technology and Advanced Studies, Chennai, Tamilnadu.
E-mail:meenakshikarthikeyan@yahoo.co.in

Abstract

Chemical graph theory plays a dominant role in the field of graph theory which involves in the study of the topological indices of Organic compound. In this paper, the structural properties of several antiviral Organic compounds in Different types of Hair Colouring DyeIndigo, Apigenin, Anthocyanin, Alizarin, Carminic.The bond measures and distance are calculated for these Organic compounds by using topological indices. These topological indices are used to be aware of benefits, and know what to do.

Hair plays a significant role in body image, and its appearance can be changed easily. The cosmetics industry has developed efficient products that can be used on healthy hair, grey hairs or act on related hair and scalp disease. Dyes beautify the hair by bleaching or colouring it briefly, for temporary periods, or permanently, depending on the dye composition.

Keywords: Bond additive measures, drug, molecular descriptors, hair coloring, Wiener indices, Szeged.

1 Introduction

Introduction to Chemical Graph Theory is a concists to the main topics and techniques in chemical graph theory, specifically the theory of topological indices. These include distance-based, degree-based, and counting-based indices[1,2].

A topological graph index, also called a molecular descriptor, is a mathematical formula that can be applied to any graph which models some molecular structure. From this indices, it is possible to analyse mathematical values and further investigate some physicochemical properties of a molecule[6]. Natural indigo was the only source of the dye until about 1900. Within a short time, however, synthetic indigo had almost completely superseded natural indigo, and today nearly all indigo produced is synthetic[18 ,19]. In the United States, the primary use for indigo is as a dye for cotton work clothes and blue jeans[5]. Over one billion pairs of jeans around the world are dyed blue with indigo. For many years indigo was used to produce deep navy-blue colors on wool. Indigo does not bond strongly to the fiber, and wear and repeated washing may slowly remove the dye Indigo is also used as a food coloring.

Indigo is a dark blue crystalline powder that melts at 390°–392°C. It is insoluble in water, alcohol, or ether but soluble in chloroform, nitrobenzene, or concentrated sulfuric acid [26, 27]. The chemical structure of indigo corresponds to the formula $C_{16}H_{10}N_2O_2$.

Apigenin is a common dietary flavonoid found in many vegetables, Chinese medicinal herbs, and fruits and has multiple physiological functions, such as antiviral, antibacterial, antioxidant, and strong anti-inflammatory activities and blood pressure reduction

Anthocyanins are polyphenol compounds that render various hues of pink, red, purple, and blue in flowers, vegetables, and fruits. Anthocyanins also play significant roles in plant propagation, ecophysiology, and plant defense mechanisms. Structurally, anthocyanins are anthocyanidins modified by sugars and acyl acids.

Anthocyanin Structure and Formula. The anthocyanin structure is derived from the flavylium ion, and its fundamental chemical formula is $C_{15}H_{11}O+$.

Apigenin is a bioflavonoid found in many fruits and vegetables, such as parsley, onions, oranges and chamomile. This flavonoid acts as an antioxidant. Research has shown that Apigenin stimulates hair growth. Biotinyl Tripeptide-1 can boost new hair growth more than 100% along with reducing hair loss by more than 50%.Apigenin is a flavonoid belonging to the flavone structural class and chemically known as 4′,5,7,-trihydroxyflavone, with molecular formula $C_{15}H_{10}O_5$.

The dyes produce red colors when used with mordants and were used for cloth, leather, and cosmetics. Lac is chemically very similar to carmine and, as the older name indicates, the insects are related to those from which carmine is obtained [26]. There are four compounds found in lac, designated laccaic acids A, B, C and D. Laccaic acid A is the most abundant. Laccaic acids A, B, and C are very similar, differing at a single point, and this is illustrated in the formulas A: $C_{26}H_{19}NO_{12}$ B: $C_{24}H_{16}O_{12}$ C: $C_{25}H_{17}NO_{13}$ D: $C_{16}H_{10}O_7$.

Carminic acid ($C_{22}H_{20}O_{13}$) is a red glucosidal hydroxyanthrapurin that occurs naturally in some scale insects, such as the cochineal, Armenian cochineal, and Polish cochineal. The insects produce the acid as a deterrent to predators. An aluminum salt of carminic acid is the coloring agent in carmine, a pigment[29, 30].

Figure 1 Apigenin $C_{15}H_{10}O_5$

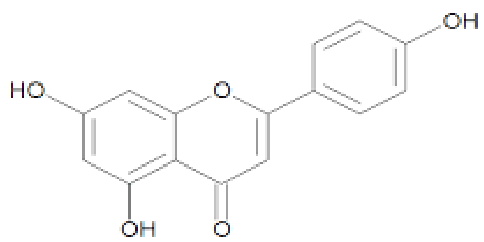


Figure 2 Anthocyanin $C_{15}H_{11}O+$

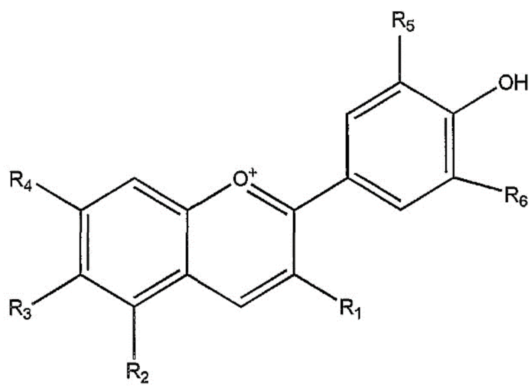


Figure 3 Laccaic acid $C_{26}H_{19}NO_{12}$

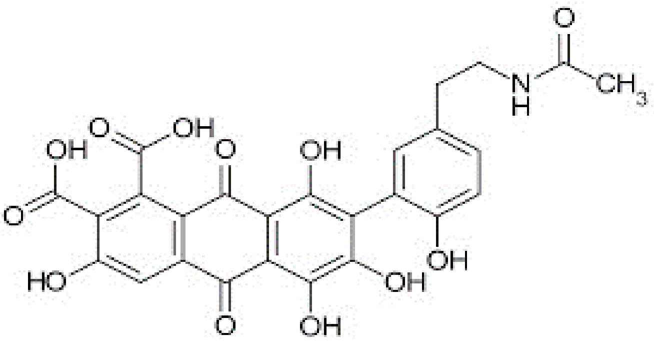
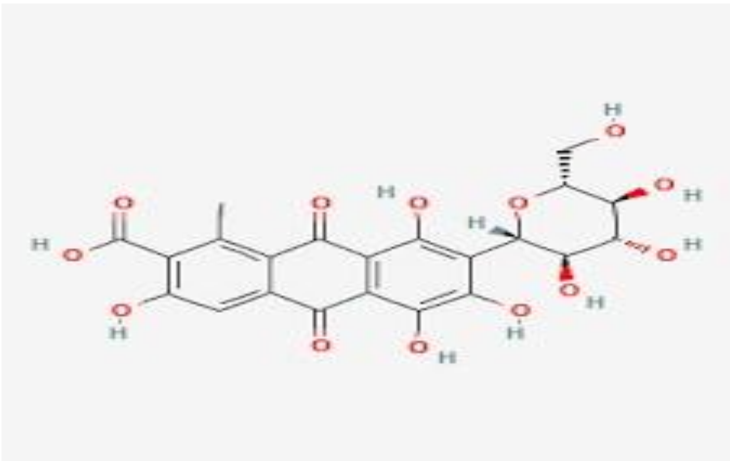


Figure 4 Carminic $C_{22}H_{20}O_{13}$



2 GRAPH PHYSICAL CONCEPTS

Let Graph = [$V(G)$, $E(G)$] be a simple graph. The degree of a vertex v is denoted as $d_G(v)$ which is characterized as the number of edges incident to v.The number of pentagons and hexagons of G are denoted by $N_p(G)$ and $N_p(G)$ respectively. For any positive integer i, we represent $N_G^i(v) = \{u \in V(G) : dg(u,v) = i\}$ as the i^{th} neighborhood of v, and thus clearly the open neighborhood of v (denoted by $N_G(v)$ is [3,4] $N_G^i(v)$. The distance between a vertex $v \in V(G)$ and an edge $e = ab \in E(G)$ denoted by $d_G(v,e)$ is defined as min $\{d_G(v, a), d_G(v, b)\}$. The distance between two edges$e = ab$ and $f = cd$ of G is defined as the minimum number of edges along a shortest (e, c)-path or a shortest (e, d)-path and denoted by $d_G(e, f)$. Foran edge $e = uv \in E(G)$ we characterize the following accompanying sets for the end vertex u:

$$N_u(e|G) = \{x \in V(G) : d_G(u,x) < d_G(v,x)\}$$

$$M_u(e|G) = \{y \in E(G) : d_G(u,y) < d_G(v,y)\}$$

In fact, $N_u(e|G)$ and $M_u(e|G)$ are the set of all vertices and edges of G which are nearer to u than to v whose cardinality is defined as $n_u(e|G)$ and $m_u(e|G)$ respectively[5,6]. The values $n_v(e|G)$ and $m_v(e|G)$ are characterized similarly. The strength-weighted graph was at first presented in Arockiaraj et al. [34] as $G_{sw} = (G, [w_v, s_v], s_e)$ where w_v is the vertex weight, s_v is the vertex strength and s_e is the edge strength. The distance between

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any two vertices in G_{sw} is denoted as $d_{G_{sw}}(u,v) = d_G(u,v)$ essentially, the sets $N_u(e|G) = N_u(e|G_{sw})$ and $M_u(e|G) = M_u(e|G_{sw})$ are described with cardinality $n_u(e|G_{sw}) = \sum_{x \in N_u(e|G_{sw})} w_v(x)$ and $m_u(e|G_{sw}) = \sum_{x \in N_u(e|G_{sw})} s_v(x) + \sum_{y \in M_u(e|G_{sw})} s_e(y)$ The value of $n_v(e|G_{sw})$ and $m_v(e|G_{sw})$ are analogous. Several topological indices (TI) for the strength-weighted graphs were studied in References [20–24] and shown in Table 1. It is to be noted that $TI(G) = TI(G_{sw})$ when $w_v = 1$, $s_v = 0$, and $s_e = 1$.

The cut method ended up being incredibly convenient when managing a distance-based graph invariants which are thusly among the focalideas of molecular graph theory. Let us recollect the concepts of isometric subgraph, partial cubes, convex subgraph and Djoković- Winkler Θ condition which are the key documentations of the cut technique[31] A graph H is supposed to be an isometric subgraph of a graph G, if for u, v c $V(H)$, $d_G(u, v) = d_H(u, v)$. The very much characterized assortment of such subgraphs of hypercubes are called partial cubes.

For any two vertices, the shortest paths between them lies inside the same subgraph then the subgraph is said to be a convex subgraph andthe condition, $d_G(s_1, s_2) + d_G(t_1, t_2) \neq d_G(s_1, t_2) + d_G(t_1, s_2)$ for two edges $e_1 = s_1t_1$ and $e_2 = s_2t_2$ is called Djoković-Winkler (Θ) relation[32,33]. This relation Θ is always reflexive, symmetric and transitive in case of partial cubes but not transitive in general. Hence the Θ partitions of the edge set of a partial cube G into classes $F_1, F_2, \ldots F_r$, called Θ-classes or convex cuts. However, its transitive closure Θ^* forms an equivalence relation in general and partitions the edge set into many convex components. A partition $\mathscr{E} = \{E_1, E_2, \ldots E_k\}$ of $E(G)$ is said to be coarser than partition $\mathscr{F}$ if each set E_i is the union of one or more Θ classes of G.

TABLE1 Topological indices of strength-weightedgraph

Topological indices	Mathematicalexpressions
Wiener	$W(G_{sw}) = \sum_{(u,v) \subseteq V(G_{sw})} W_v(u) W_v(v) dG_{sw}(u,v)$
Edge- Wiener	$W_e(G_{sw}) = \sum_{(u,v) \subseteq V(G_{sw})} S_v(u) S_v(v) dG_{sw}(u,v) + W_e(G_{sw}) + \sum_{(e,f) \subseteq E(G_{sw})} S_e(e) S_e(f) D_{G_{sw}}(e,f) + \sum_{u \in V(G_{sw})} \sum_{f \in E(G_{sw})} S_v(u) S_e(f) dG_{sw}(u,f)$
Szeged	$Sz_v(G_{sw}) = \sum_{e=uv \in E(G_{sw})} S_e(e) n_u(e|G_{sw}) n_v(e|G_{sw})$
Edge- Szeged	$Sz_e(G_{sw}) = \sum_{e=uv \in E(G_{sw})} S_e(e) m_u(e|G_{sw}) m_v(e|G_{sw})$
Padmakar- lvan	$Pl(G_{sw}) = \sum_{e=uv \in E(G_{sw})} S_e(e) \left[m_u(e|G_{sw}) + m_v(e|G_{sw})\right]$
Mostar	$Mo(G_{sw}) = \sum_{e=uv \in E(G_{sw})} S_e(e) \left[n_u(e|G_{sw}) - n_v(e|G_{sw})\right]$
Edge- Mostar	$Mo_e(G_{sw}) = \sum_{e=uv \in E(G_{sw})} S_e(e) \left[m_u(e|G_{sw}) - m_v(e|G_{sw})\right]$

3 TOPOLOGICAL INDICES BASED ON DISTANCE

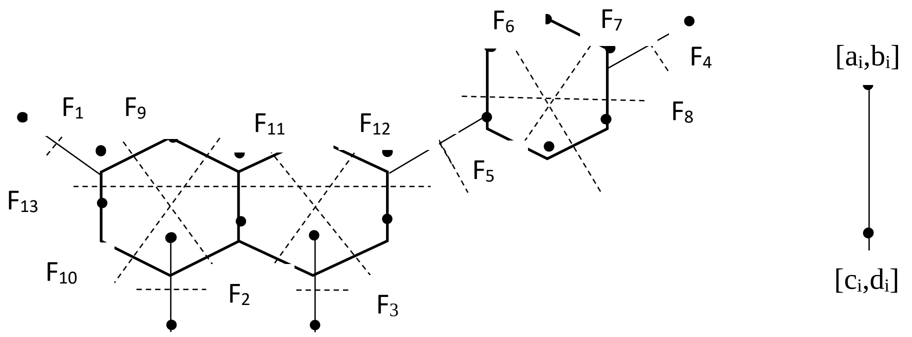
In this section is to compute several distance-based and bond additive topological indices of chemical compounds considered in our study. Inthe sequence, we assume that the vertex strength-weighted values of a quotient graph for the convex cut F_i of G as $[a_i, b_i]$, $[c_i, d_i]$ and edge strengthas e_i such that $c_i = |V(G)| - a_i$ and $d_i = |E(G)| - b_i - e_i$.

Theorem:1

Let G_1 be apigenin compound then $W(G_1) = 788$, $W_e(G_1) = 216$, $Sz_v(G_1) = 1509$, $Sz_e(G_1) = 406$, $Pl(G_1) = 244$, $Mo(G_1) = 212$.

Proof:

The apigenin compound has 20 vertices and 22 edges.Let $\{Fi : 1 \le i \le 4\}$ be the different convex cut of G_1 and the corresponding quotient graph which are characterizein Figure 1. The strength-weighted values G_1/F_i are presentedinTable1andinaddition,e_i=1,1≤i≤5;e_i=2,6≤i≤12;e_{13}=3.By using simple calculation mathematical method based on cut method.we obtain the following the topological indices are



(A) (B)

FIGURE:5 (A) Different cuts of Apigenin G_1,(B) quotientgraphG_1/F_i

TABLE1 Strength-weighted valuesofquotientgraphG_1/F_i

F_i	1≤i≤4	5	6	7	8	9	10	11	12	13
a_i	1	4	4	4	7	5	4	7	9	10
b_i	0	3	3	3	7	4	3	6	9	9

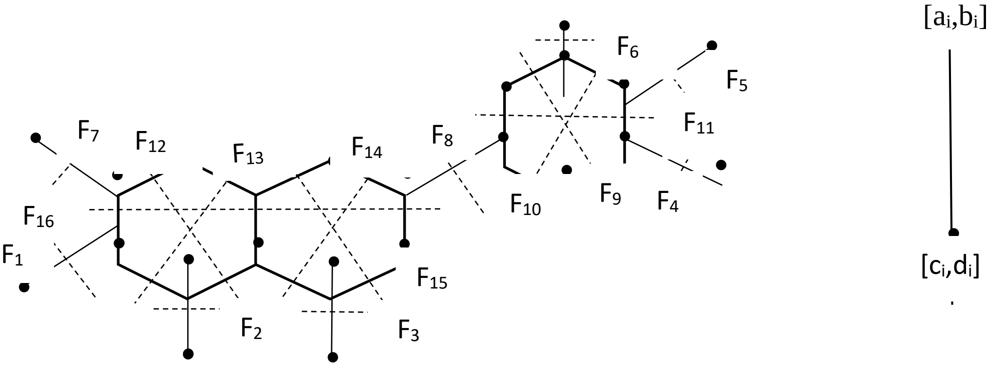
we find the topological indices as $W(G_1) = \sum_{i=1}^{13} a_i c_i = 788$, $W_e(G_1) = \sum_{i=1}^{13} b_i d_i = 171$, $Sz_v(G_1) = \sum_{i=1}^{13} e_i a_i c_i = 1509$, $Sz_e(G_1) = \sum_{i=1}^{13} e_i b_i d_i = 1077$, $Pl(G_1) = \sum_{i=1}^{13} e_i (b_i + d_i) = 443$, $Mo(G_1) = \sum_{i=1}^{13} e_i |a_{i-} c_i| = 217$.

Theorem:2

Let G_2 be Anthocyanin compound then $W(G_1) = 788$, $W_e(G_1) = 216$, $Sz_v(G_1) = 1509$, $Sz_e(G_1) = 406$, $Pl(G_1) = 244$, $Mo(G_1) = 212$.

Proof:

The Anthocyanin compound has 23 vertices and 25 edges.Let $\{Fi : 1 \le i \le 7\}$ be the different convex cut of of G_2 and the corresponding quotient graph which are characterizein Figure 2. The strength-weighted valuesG_2/F_i are presented inTable2 and in addition, e_i=1,1≤i≤8; e_i=2, 8≤i≤12; e_{13}=3.



(A) **(B)**

FIGURE:6 (A) Different cuts of Apigenin G_2,(B) quotientgraphG_2/F_i

TABLE :2 Strength-weighted values of quotientgraph G_2/F_i

F_i	1≤i≤7	8	9	10	11	12	13	14	15	16
a_i	1	9	6	5	5	6	5	10	11	8
b_i	0	9	5	4	4	5	4	10	11	7

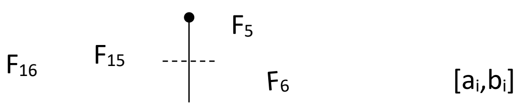
we find the topological indices as $W(G_1) = \sum_{i=1}^{16} a_i c_i = 1224$, $W_e(G_1) = \sum_{i=1}^{16} b_i d_i = 216$, $Sz_v(G_1) = \sum_{i=1}^{16} e_i a_i c_i = 2108$, $Sz_e(G_1) = \sum_{i=1}^{16} e_i b_i d_i = 406$, $Pl(G_1) = \sum_{i=1}^{16} e_i (b_i + d_i) = 244$, $Mo(G_1) = \sum_{i=1}^{16} e_i |a_{i-} c_i| = 226.$

Theorem:3

Let G_3 be Laccaic acids compound then $W(G_1) = 4007$, $W_e(G_1) = 3762$, $Sz_v(G_1) = 6719$, $Sz_e(G_1) = 7066$, $Pl(G_1) = 1600$, $Mo(G_1) = 1024$.

Proof:

The Laccaic acids compound has 39 vertices and 41 edges.Let $\{Fi : 1 \le i \le 4\}$ be the different convex cut of of G_3 and the corresponding quotient graph which are characterizein Figure 3.The strength eightedvaluesG_3/F_i are represented inTable 3and ina ddition,e_i=1,1≤i≤5;e_i=2,6≤i≤12;e_{13}=3.



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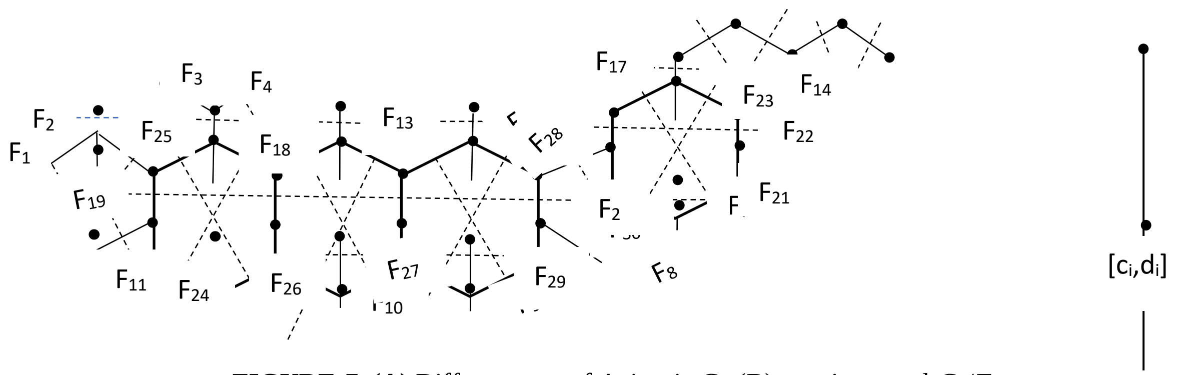


FIGURE:7 (A) Different cuts of Apigenin G_3,(B) quotientgraphG_3/F_i

TABLE :3 Strength-weighted values of quotientgraph G_3/F_i

FFi	1≤i≤13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
a_i	1	3	.4	5	6	3	3	4	9	9	9	10	7	15	15	22	22	11
b_i	0	2	3	4	5	2	2	3	8	8	8	9	6	15	15	22	22	10

Now we find the topological indices as $W(G_1)=\sum_{i=1}^{30} a_i c_i = 4007$, $W_e(G_1)=\sum_{i=1}^{30} b_i d_i = 3762$, $Sz_v(G_1)=\sum_{i=1}^{30} e_i a_i c_i = 6719$, $Sz_e(G_1)=\sum_{i=1}^{30} e_i b_i d_i = 7066$, $Pl(G_1)=\sum_{i=1}^{30} e_i(b_i+d_i)=1600$, $Mo(G_1)=\sum_{i=1}^{30} e_i\left|a_{i-}c_i\right|=1024$.

Theorem:4
Let G_4 be Carminic compound then $W(G_1)=3012$, $W_e(G_1)=2272$, $Sz_v(G_1)=5768$, $Sz_e(G_1)=3688$, $Pl(G_1)=5440$, $Mo(G_1)=919$.

Proof:
The Carminic compound has 34 vertices and 37 edges.Let $\{Fi : 1 \le i \le 4\}$ be the different convex cut of of G_4 and the corresponding quotient graph which are characterizein Figure 4. Thestrength-weightedvaluesG_4/F_i are represented inTable2 and in addition,e_i=1,1≤i≤15;e_i=2,16≤i≤24;e_{25}=4.

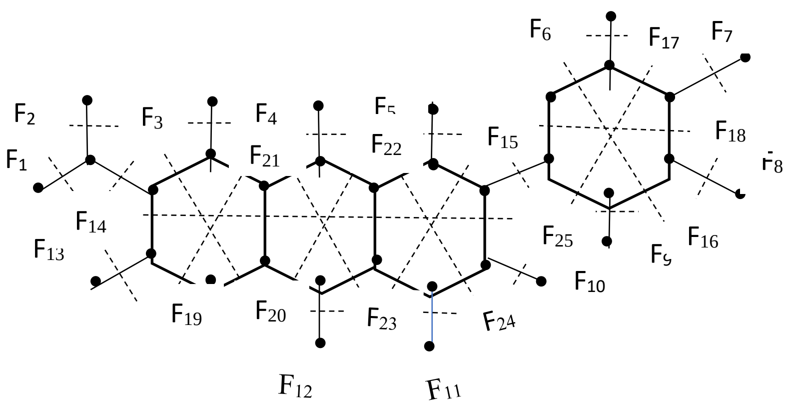


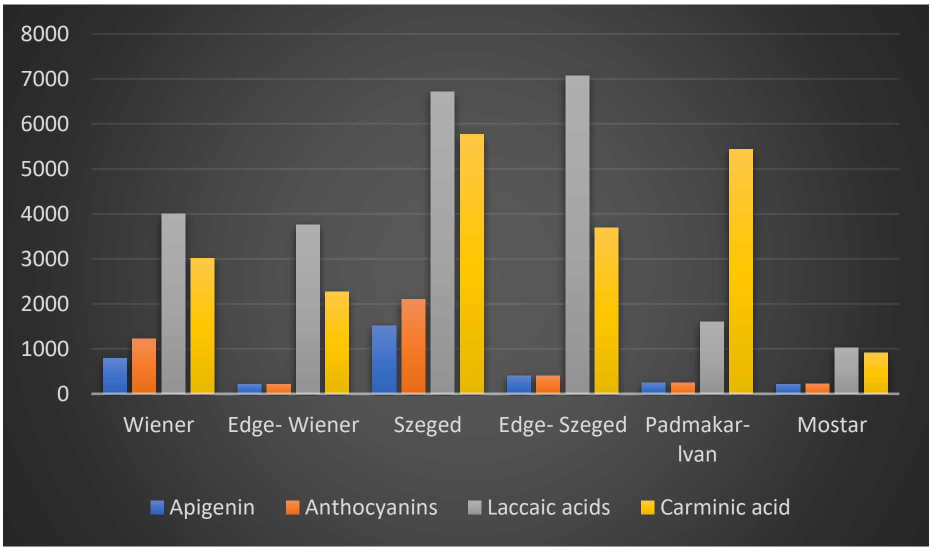
FIGURE:8 (A) Different cuts of Apigenin G_4,(B) quotientgraphG_4/F_i

TABLE :4 Strength-weighted values of quotientgraph G_4/F_i

Fi	1≤i≤13	14	15	16	17	18	19	20	21	22	23	24	25
a_i	1	3	10	6	6	5	8	7	13	13	19	19	11
b_i	0	2	10	5	5	4	7	6	14	14	21	21	10

we find the topological indices as $W(G_1)=\sum_{i=1}^{25} a_i c_i = 3012$, $W_e(G_1)=\sum_{i=1}^{25} b_i d_i = 2272$, $Sz_v(G_1)=\sum_{i=1}^{25} e_i a_i c_i = 5768$, $Sz_e(G_1)=\sum_{i=1}^{25} e_i b_i d_i = 3688$, $Pl(G_1)=\sum_{i=1}^{25} e_i (b_i + d_i) = 5440$, $Mo(G_1)=\sum_{i=1}^{25} e_i |a_{i-} c_i| = 919$.

FIGURE:9 A graphical representation of topological indices of different hair colouring compounds



4 CONCLUSION

In this paper using simple calculation of mathematical method based on cut method.we obtain the following the topological indices are Wiener Edge- Wiener Szeged Edge- Szeged Padmakar- Ivan for strength-weighted graphs with respect to Djoković- Winkler Θ condition.Apigenin is a flavon which is considered to be safe, even in a high dose, and so far no toxicity of this molecule has been reported A typical anthocyanin pigment appears red in acid, carminic acid may cause allergic reactions and even anaphylactic shock to a sensitive subset of populations. These types of chemicals side effects may occur in people who are allergic to the insect proteins and can develop after direct contact, inhalation or consumption. Some carmine allergy symptoms that may occur include face swelling, rash, redness and wheezing.

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