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Degree-Based Topological Indices and M - Polynomial of Famotidine

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Abstract:
Famotidine, also known as Pepcid, is a drug used to treat acid reflux and heartburn caused by food or drink. In this study, various topological indices of chemical graph theory were calculated to determine the physical and chemical properties of the studied molecules. These indices include the first and second Zagreb indices, the first and second Zagreb eccentricity indices, the first and second location indices, Famotidine Sanskruti indices and other topological indices.
Keywords: topological, reflux, heartburn, Famotidine

Introduction:

Famotidine, manufactured by Yamanouchi Pharmaceutical Co. and licensed by Merck & Co., is a powerful drug used to treat acid reflux and heartburn caused by food or drink. It is commonly known by its brand name, Pepcid. Famotidine has been on the market since the mid-1980s and is currently managed through a joint venture between Merck and Johnson & Johnson.

The chemical structure of Famotidine involves replacing the imidazole ring of Cimetidine with a 2-guanidinothiazole ring. Comparative studies have shown that Famotidine is nine times more potent than Ranitidine and 32 times more potent than Cimetidine in treating acid reflux and heartburn. It was first introduced to the market in 1981.

Over the years, Famotidine has undergone further developments. In 1999, oral dispersants were introduced under the brand name Pepcid RPD. In 2001, the brand acquired Fluxid (Schwarz) and Quamatel (Gedeon Richter Ltd.). In the United States and Canada, a combination drug called Pepcid Complete, which includes Famotidine and Antacid, is available in tablet form for immediate relief of heartburn associated with high stomach acid. In the UK, this drug used to be called Pepcid Two until it was discontinued in April 2015.

Famotidine has a bioavailability of only 50% due to its short intestinal retention time. However, when used with Antacids, the intestinal retention time is prolonged, leading to improved transfer of the drug into the region and receptors of the parietal skin, thereby increasing its bioavailability. Researchers are currently investigating tablet formulations that use different gastroprotective drug delivery systems, including floating tablets, to further improve the bioavailability of Famotidine.

Famotidine is primarily used to treat stomach problems associated with acid reflux. It works by inhibiting the production of stomach acid through its medicinal properties. The drug is available in both prescription and over-the-counter forms.

The FDA has approved Famotidine for the treatment of the following conditions:

1. Duodenal ulcers in adults and children
2. Peptic ulcers
3. Gastroesophageal reflux disease (GERD)

Famotidine is also used to treat hypersecretory conditions in adults, but it is only available by prescription. In addition, the FDA has approved Famotidine for the treatment and prevention of heartburn caused by gastroesophageal reflux disease in both adults and children. It can also be used off-label, meaning medical professionals can adjust the patient's treatment as necessary to achieve the desired results, taking into account the indications, procedures, administration methods, significant adverse reactions, contraindications, monitoring, and Famotidine toxicity.

The chemical formula of Famotidine is $C_8H_{15}N_7O_2S_3$. The 2D and 3D molecular structures of Famotidine are shown in Figure 1 and 2 respectively.

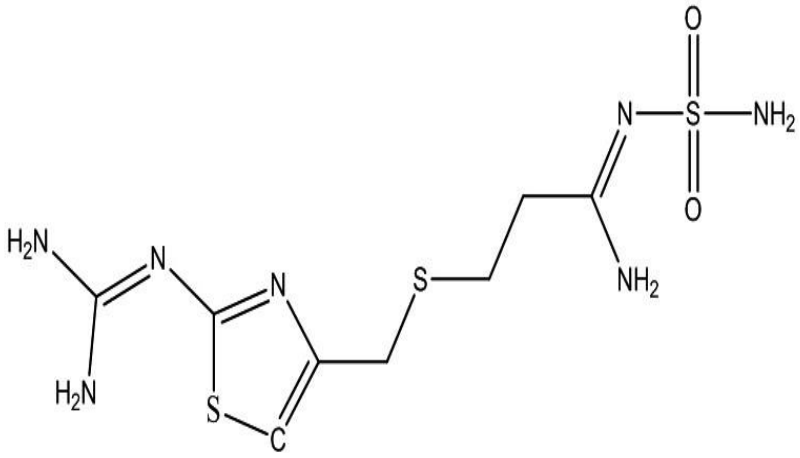

Figure 1: 2D molecular structures of Famotidine

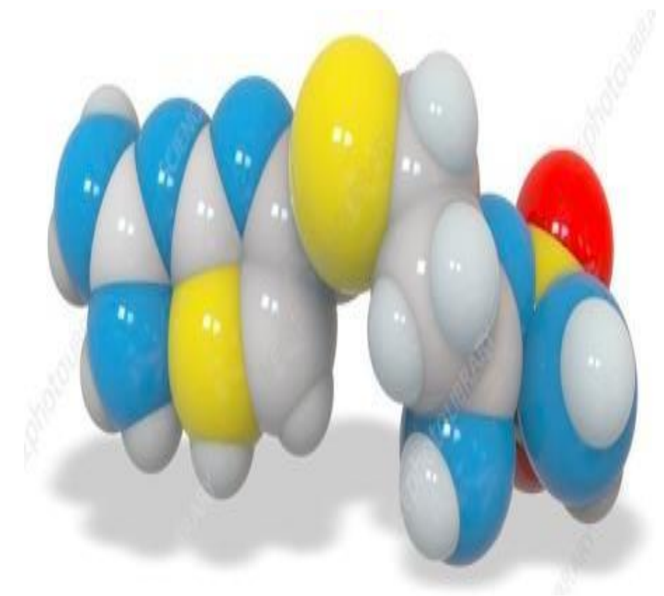

Figure 2: 3D molecular structures of Famotidine

Topological graph indices, or molecular descriptors, are mathematical formulas applied to graphs representing molecular structures. These indices provide valuable information about a molecule's structure and properties. In this context, atoms are represented as vertices, and bonds between atoms are represented as edges. Various types of topological matrices, such as distance or adjacency matrices, can be used to describe the connections between atoms in a molecule. These matrices are then manipulated mathematically to generate a single numerical value known as a graph invariant, graph-theoretical index, or topological index. These indices can be useful in various areas of chemistry, such as predicting molecular properties, drug design, and structure-activity relationships. By analysing the values of topological indices, researchers can gain insights into a molecule's reactivity, stability, solubility, and other important characteristics. It's important to note that different topological indices focus on different aspects of a molecule's structure, and their interpretations may vary depending on the specific context or application.

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Let $G = (\varphi, \psi)$ be a molecular graph, then the topological indices can be considered as a function of real values $\chi: G \to R$ and $\phi(G)$can be represented as a vertex set and $\psi(G)$ can be represented as an edge set. The degree of a vertex $a \epsilon \phi(G)$ is denoted by r_a which is the number of edges that are incident to the vertex.

Table 1: Index Name and definition.

R4c4r Index Name	Definition
First and Second Zagreb	$M_1(G) = \sum_{e\in\psi(G)} (r_a + r_b)$ $M_2(G) = \sum_{e\in\psi(G)} (r_a r_b)$
Hyper Zagreb	$HM(G) = \sum_{e\in\psi(G)} (r_a + r_b)^2$
Harmonic	$H(G) = \sum_{e\in\psi(G)} \frac{2}{r_a + r_b}$
First and Second Entire Zagreb	$M_1^\theta(G) = \sum_{\gamma\in\phi(G)\cup\psi(G)} (r_\gamma)^2$ $M_2^\theta(G) = \sum_{\{\beta,\gamma\}\in A(G)} (r_\beta).(r_\gamma)$
First and Second Locating	$M_1^L(G) = \sum_{a_i\in\phi(G)} (\vec{a}_i)^2$ $M_2^L(G) = \sum_{e\in\psi(G)} (\vec{r}_a).(\vec{r}_b)$
Sanskruti	$S(G) = \sum_{e\in\psi(G)} \left(\frac{S_G(a)S_G(b)}{S_G(a)+S_G(b)-2}\right)^3$
First and Second Eccentricity Zagreb	$E_1(G) = \sum_{a_i\in\phi(G)} (ld)_i^2$ $E_2(G) = \sum_{e\in\psi(G)} (ld)_i(ld)_j$
First and Second-Degree Eccentricity Zagreb	$DE_1(G) = \sum_{a_i\in\phi(G)} ((ld)_i + d_i)^2$ $DE_2(G) = \sum_{e\in\psi(G)} ((ld)_i + d_i)((ld)_j + d_j)$
Atom Bond Connectivity	$ABC(G) = \sum_{e\in\psi(G)} \sqrt{\frac{r_a + r_b - 2}{r_a r_b}}$
Randic	$R(G) = \sum_{e\in\psi(G)} \frac{1}{\sqrt{r_a r_b}}$
Sum Connectivity	$S(G) = \sum_{e\in\psi(G)} \frac{1}{\sqrt{r_a + r_b}}$
Geometric Arithmetic	$GA(G) = \sum_{e\in\psi(G)} \frac{2\sqrt{r_a r_b}}{r_a + r_b}$
Fifth Geometric Arithmetic	$GA_5(G) = \frac{2\sqrt{S_a S_b}}{S_a + S_b}$
Fourth Atom Bond Connectivity	$ABC_4(G) = \sum_{e\in\psi(G)} \sqrt{\frac{S_a + S_b - 2}{S_a S_b}}$

Main Proof and Results:

Theorem 2.1

The First and Second Zagreb indices of $C_8H_{15}N_7O_2S_3M_1$ are 94 and 99 respectively.

Proof:

We partition the edges of $C_8H_{15}N_7O_2S_3$ into edges of the type $E_{(d_u\, d_v)}$ where uv is an edge. In $C_8H_{15}N_7O_2S_3$, we get edges of the type

Edge Partition	Number of Edges
$\lvert E_{1,3}\rvert$	3
$\lvert E_{2,3}\rvert$	9
$\lvert E_{2,2}\rvert$	4
$\lvert E_{1,4}\rvert$	3
$\lvert E_{2,4}\rvert$	1

We know that, $M_1(G) = \sum_{e\in\psi(G)} \quad (r_a + r_b)$

$$M_2(G) = \sum_{e\in\psi(G)} \quad (r_a r_b)$$

M_1 $(C_8H_{15}N_7O_2S_3)$ = $|E_{1,3}|(1+3) + |E_{2,3}|\ (2+3) + |E_{2,2}|\ (2+2) + |E_{1,4}|\ (1+4) + |E_{2,4}|\ (2+4)$

$= 3(4) + 9\ (5) + 4(4) + 3(5) + 1\ (6) = 94$

M_2 $(C_8H_{15}N_7O_2S_3)$ = $|E_{1,3}|(1.3) + |E_{2,3}|\ (2.3) + |E_{2,2}|\ (2.2) + |E_{1,4}|\ (1.4) + |E_{2,4}|\ (2.4)$

$= 3(3) + 9\ (6) + 4(4) + 3(4) + 1\ (8) = 99$

Theorem 2.2

The Hyper Zagreb index of $C_8H_{15}N_7O_2S_3M_1$ is 448.

Proof:

We know that, $HM(G) = \sum_{e\in\psi(G)} \quad (r_a + r_b)^2$

HM $(C_8H_{15}N_7O_2S_3)$ = $|E_{1,3}|(1+3)^2 + |E_{2,3}|\ (2+3)^2 + |E_{2,2}|\ (2+2)^2 + |E_{1,4}|\ (1+4)^2 + |E_{2,4}|\ (2+4)^2$

$=3\ (16) + 9\ (25) + 4\ (16) + 3\ (25) + 1\ (36) = 448$

Theorem 2.3

The Harmonic index of $C_8H_{15}N_7O_2S_3M_1$ is 8.6.

Proof:

We know that, $H(G) = \sum_{e\in\psi(G)} \frac{2}{c_a + c_b}$

H$(C_8H_{15}N_7O_2S_3)$ = $|E_{1,3}|\frac{2}{4} + |E_{2,3}|\frac{2}{5} + |E_{2,2}|\frac{2}{4} + |E_{1,4}|\frac{2}{5} + |E_{2,4}|\frac{2}{6}$

$= 8.6$

Theorem 2.4

The Randic index of $C_8H_{15}N_7O_2S_3M_1$ is 9.26.

Proof:

We know that, $R(G) = \sum_{e\in\psi(G)} \frac{1}{\sqrt{c_a c_b}}$

R$(C_8H_{15}N_7O_2S_3)$ = $|E_{1,3}|\frac{1}{\sqrt{3}} + |E_{2,3}|\frac{1}{\sqrt{6}} + |E_{2,2}|\frac{1}{\sqrt{4}} + |E_{1,4}|\frac{1}{\sqrt{4}} + |E_{2,4}|\frac{1}{\sqrt{8}}$

$= 9.26$

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Theorem 2.5

The Sum Connectivity index of $C_8H_{15}N_7O_2S_3M_1$ is 9.28.

Proof:

We know that,

$$S(G) = \sum_{e\in\psi(G)} \frac{1}{\sqrt{c_a+c_b}}$$

$$S(C_8H_{15}N_7O_2S_3) = |E_{1,3}| \frac{1}{\sqrt{4}} + |E_{2,3}| \frac{1}{\sqrt{5}} + |E_{2,2}| \frac{1}{\sqrt{4}} + |E_{1,4}| \frac{1}{\sqrt{5}} + |E_{2,4}| \frac{1}{\sqrt{6}}$$

$$= 9.28$$

Theorem 2.6

The Geometric Arithmetic index of $C_8H_{15}N_7O_2S_3M_1$ is 14.63.

Proof:

We know that,

$$GA(G) = \sum_{e\in\psi(G)} \frac{2\sqrt{c_a c_b}}{c_a+c_b}$$

$$GA(C_8H_{15}N_7O_2S_3) = |E_{1,3}| \frac{2\sqrt{3}}{4} + |E_{2,3}| \frac{2\sqrt{6}}{5} + |E_{2,2}| \frac{2\sqrt{4}}{4} + |E_{1,4}| \frac{2\sqrt{4}}{5} + |E_{2,4}| \frac{2\sqrt{8}}{6}$$

$$= 14.63$$

Theorem 2.7

The Fourth Atom Bond Connectivity index of $C_8H_{15}N_7O_2S_3M_1$ is 11.52.

Proof:

We know that, $ABC_4(G) = \sum_{e\in\psi(G)} \sqrt{\frac{S_a+S_b-2}{S_aS_b}}$

$$ABC_4(C_8H_{15}N_7O_2S_3) = \sqrt{\frac{3+4-2}{12}} + \sqrt{\frac{3+4-2}{12}} + \sqrt{\frac{4+6-2}{24}} + \sqrt{\frac{6+6-2}{36}} + \sqrt{\frac{6+5-2}{30}}$$
$$+ \sqrt{\frac{5+5-2}{25}} + \sqrt{\frac{6+5-2}{30}} + \sqrt{\frac{6+6-2}{36}} + \sqrt{\frac{6+6-2}{36}} + \sqrt{\frac{6+5-2}{30}}$$
$$+ \sqrt{\frac{4+5-2}{20}} + \sqrt{\frac{4+4-2}{16}} + \sqrt{\frac{4+5-2}{20}} + \sqrt{\frac{5+5-2}{25}} + \sqrt{\frac{5+3-2}{15}}$$
$$+ \sqrt{\frac{5+7-2}{35}} + \sqrt{\frac{5+4-2}{20}} + \sqrt{\frac{5+4-2}{20}} + \sqrt{\frac{5+7-2}{35}} + \sqrt{\frac{5+4-2}{20}}$$

$ABC_4(C_8H_{15}N_7O_2S_3) = 11.52$

Theorem 2.8

The Fifth Geometric Arithmetic index of $C_8H_{15}N_7O_2S_3M_1$ is 22.81.

Proof:

We know that, $GA_5(G) = \frac{2\sqrt{S_aS_b}}{S_a+S_b}$

$$GA_5(C_8H_{15}N_7O_2S_3) = \frac{2\sqrt{12}}{7} + \frac{2\sqrt{12}}{7} + \frac{2\sqrt{24}}{10} + \frac{2\sqrt{36}}{12} + \frac{2\sqrt{30}}{11} + \frac{2\sqrt{25}}{10} + \frac{2\sqrt{30}}{11}$$
$$+ \frac{2\sqrt{36}}{12} + \frac{2\sqrt{36}}{12} + \frac{2\sqrt{30}}{11} + \frac{2\sqrt{20}}{9} + \frac{2\sqrt{16}}{8} + \frac{2\sqrt{20}}{9} + \frac{2\sqrt{25}}{10}$$
$$+ \frac{2\sqrt{15}}{8} + \frac{2\sqrt{35}}{12} + \frac{2\sqrt{20}}{9} + \frac{2\sqrt{20}}{9} + \frac{2\sqrt{15}}{8} + \frac{2\sqrt{20}}{9}$$

$ABC_4(C_8H_{15}N_7O_2S_3) = 22.81$

Theorem 2.9

The Atom Bond Connectivity of $C_8H_{15}N_7O_2S_3M_1$ is 14.95.

Proof:

We know that, $ABC(G) = \sum_{e\in\psi(G)} \sqrt{\frac{c_a+c_b-2}{c_ac_b}}$

$$ABC(C_8H_{15}N_7O_2S_3) = |E_{1,3}| \sqrt{\frac{1+3-2}{3}} + |E_{2,3}| \sqrt{\frac{2+3-2}{6}} + |E_{2,2}| \sqrt{\frac{2+2-2}{4}} + |E_{1,4}| \sqrt{\frac{1+4-2}{4}} + |E_{2,4}| \sqrt{\frac{2+4-2}{8}}$$

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ABC ($C_8H_{15}N_7O_2S_3$) = 14.95

Theorem 2.10

The First and Second Entire Zagreb indices of $C_8H_{15}N_7O_2S_3M_1$ are 246 and 357 respectively.

Proof:

We know that, $M_1^{\theta}(G) = \sum_{\gamma \in \phi(G) \cup \psi(G)} (r_\gamma)^2$

$M_2^{\theta}(G) = \sum_{\{\beta,\gamma\} \in A(G)} (r_\beta).\ (r_\gamma)$

M_1^{θ} ($C_8H_{15}N_7O_2S_3$) = 246

Similarly,

$A(G)$ set of all $\{\beta,\gamma\} \ni \{\beta,\gamma\} \in \phi(G) \cup \psi(G)$ i.e $\{\beta,\gamma\}$ are adjacent or incident to each other.

$M_2^{\theta}(G) = \sum_{\beta \text{ is either adjacent or incident to } \gamma} (r_\beta).\ (r_\gamma)$

M_2^{θ} ($C_8H_{15}N_7O_2S_3$) = 357

Theorem 2.10

The First and Second Zagreb Locating indices of $C_8H_{15}N_7O_2S_3M_1$ are 15,941 and 14,617 respectively.

Proof:

We find

$a_1 = (0,2,1,2,3,4,5,6,4,6,7,8,9,10,11,11,12,13,13,13)$,
$a_2 = (2,0,1,2,3,4,5,5,4,6,7,8,9,10,11,11,12,13,13,13)$,
$a_3 = (1,1,0,1,2,3,4,4,3,5,6,7,8,9,10,10,11,12,12,12)$,
$a_4 = (2,2,1,0,1,2,3,3,2,4,5,6,7,8,9,10,10,11,11,11)$,
$a_5 = (3,3,2,1,0,1,2,2,1,3,4,5,6,7,8,8,9,10,10,10)$,
$a_6 = (4,4,3,2,1,0,1,2,2,3,4,5,6,7,8,8,9,10,10,10)$,
$a_7 = (5,5,4,3,2,1,0,1,2,2,3,4,5,6,7,7,8,9,9,9)$,
$a_8 = (5, 5,4,3,2,2,1,0,1,1,2,3,4,5,6,6,7,8,8,8)$,
$a_9 = (4,4,3,2,1,2,2,1,0,2,3,4,5,6,7,7,8,9,9,9)$,
$a_{10} = (6,5,5,4,3,3,2,1,2,0,1,2,3,4,5,5,6,7,7,7)$,
$a_{11} = (7,7,6,5,4,4,3,2,3,1,0,1,2,3,4,4,5,6,6,6)$,
$a_{12} = (8,8,7,6,5,5,4,3,4,2,1,0,1,2,3,3,4,5,5,5)$,
$a_{13} = (9,9,8,7,6,6,5,4,5,3,2,1,0,1,2,2,3,4,4,4)$,
$a_{14} = (10,10,9,8,7,7,6,5,6,4,3,2,1,0,1,1,2,3,3,3)$,
$a_{15} = (11,11,10,9,8,8,7,6,7,5,4,3,2,1,0,2,3,4,4,4)$,
$a_{16} = (11,11,10,9,8,8,7,6,7,5,4,3,2,1,2,0,1,2,2,2)$,
$a_{17} = (12,12,11,10,9,9,8,7,8,6,5,4,3,2,3,1,0,1,1,1)$,
$a_{18} = (13,13,12,11,10,10,9,8,9,7,6,5,4,3,4,2,1,0,2,2)$,
$a_{19} = (13,13,12,11,10,10,9,8,9,7,6,5,4,3,4,2,1,2,0,2)$,
$a_{20} = (13,13,12,11,10,10,9,8,9,7,6,5,4,3,4,2,1,2,2,0)$.

We know that,

$M_1^{\ell}(G) = \sum_{a_i \in \phi(G)} (\vec{a_i})^2$

$a_1^{\ 2} = 1334$, $a_2^{\ 2} = 1323$, $a_3^{\ 2} = 1065$, $a_4^{\ 2} = 870$, $a_5^{\ 2} = 677$
$a_6^{\ 2} = 699$, $a_7^{\ 2} = 580$, $a_8^{\ 2} = 453$, $a_9^{\ 2} = 550$, $a_{10}^{\ 2} = 392$
$a_{11}^{\ 2} = 393$, $a_{12}^{\ 2} = 423$, $a_{13}^{\ 2} = 493$, $a_{14}^{\ 2} = 603$, $a_{15}^{\ 2} = 801$
$a_{16}^{\ 2} = 757$, $a_{17}^{\ 2} = 951$, $a_{18}^{\ 2} = 1193$, $a_{19}^{\ 2} = 1191$, $a_{20}^{\ 2} = 1193$

$M_1^{\ell}(C_8H_{15}N_7O_2S_3) = 15{,}941$

Similarly, we compute the second Zagreb locating indices

$M_2^{\ell}(G) = \sum_{e \in \psi(G)} (\vec{r}_{\vec{a}}).(\vec{r}_{\vec{b}})$

$M_2^{\ell}(C_8H_{15}N_7O_2S_3) = 14{,}617$

The proof is complete.

Theorem 2.11

The Sanskruti indices of $C_8H_{15}N_7O_2S_3M_1$ is 604.994.

Proof:

We know that,

$$S(G) = \sum_{e\in\psi(G)} \left(\frac{S_G(a)S_G(b)}{S_G(a)+S_G(b)-2}\right)^3 \text{--------- (i)}$$

$$S_G(a) = \sum_{ag N(a)} r_b \text{----------------------------------(ii)}$$

Using Equation (ii), we get

$S_{a_1} = 3$, $S_{a_2} = 3$, $S_{a_3} = 4$, $S_{a_4} = 6$, $S_{a_5} = 6$, $S_{a_6} = 5$, $S_{a_7} = 5$, $S_{a_8} = 6$, $S_{a_9} = 6$, $S_{a_{10}} = 5$, $S_{a_{11}} = 4$, $S_{a_{12}} = 4$, $S_{a_{13}} = 5$, $S_{a_{14}} = 5$, $S_{a_{15}} = 3$, $S_{a_{16}} = 7$, $S_{a_{17}} = 5$, $S_{a_{18}} = 4$, $S_{a_{19}} = 4$, $S_{a_{20}} = 4$.

$$S(C_8H_{15}N_7O_2S_3) = 604.99$$

Theorem 2.12

The First and Second Eccentricity Zagreb of $C_8H_{15}N_7O_2S_3M_1$ are 2265 and 2121 respectively.

Proof:

We know that,

$$(ld)_i = max_{a_i\in\phi(G)} r_G(a_i, a_j)$$

By using above equation, we find the largest distance between the vertices.

$(ld)_1 = 13$, $(ld)_2 = 13$, $(ld)_3 = 12$, $(ld)_4 = 11$, $(ld)_5 = 10$, $(ld)_6 = 10$, $(ld)_7 = 9$, $(ld)_8 = 8$, $(ld)_9 = 9$, $(ld)_{10} = 7$, $(ld)_{11} = 7$, $(ld)_{12} = 8$, $(ld)_{13} = 9$, $(ld)_{14} = 10$, $(ld)_{15} = 11$, $(ld)_{16} = 11$, $(ld)_{17} = 12$, $(ld)_{18} = 13$, $(ld)_{19} = 13$, $(ld)_{20} = 13$.

The First and Second Eccentricity Zagreb indices is

$$E_1(G) = \sum_{a_i\in\phi(G)} (ld)_i^2$$

$$E_2(G) = \sum_{e\in\psi(G)} (ld)_i(ld)_j$$

$$E_1(C_8H_{15}N_7O_2S_3) = 5 * 13^2 + 2 * 12^2 + 3 * 11^2 + 3 * 10^2 + 3 * 9^2 + 2 * 8^2 + 2 * 7^2 = 2265$$

Similarly, we compute the Second Eccentricity Zagreb index

$$E_2(C_8H_{15}N_7O_2S_3) = 2121$$

The proof is complete.

Theorem 2.13

The Zagreb degree Eccentricity indices of $C_8H_{15}N_7O_2S_3M_1$ are 3090 and 3570 respectively.

Proof:

We know that,

$$DE_1(G) = \sum_{a_i\in\phi(G)} ((ld)_i + d_i)^2$$

$$DE_2(G) = \sum_{e\in\psi(G)} ((ld)_i + d_i)((ld)_j + d_j)$$

By using the above equations, we get the required result.

$$DE_1(C_8H_{15}N_7O_2S_3) = 3090$$

$$DE_2(C_8H_{15}N_7O_2S_3) = 3570$$

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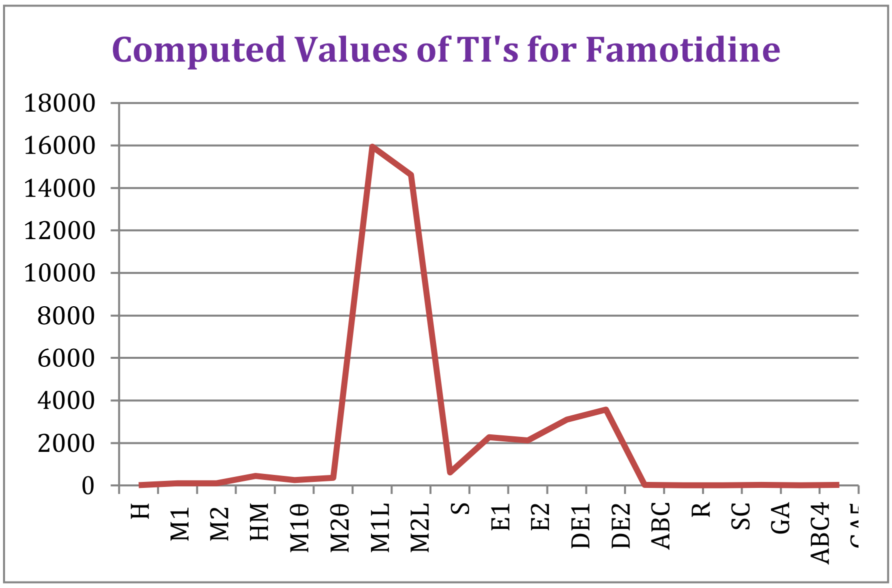
Graph Analysis:



3. M - polynomial of famotidine drugs:

The M-polynomial is a mathematical polynomial that can be used to calculate various degree-based topological indices of a molecular graph. It is a general polynomial that provides formulae that closely approximate these indices. The M-polynomial is defined as follows:

$$M(G; a, b) = \sum_{r \leq s} \eta_{rs}(G) a^r b^s$$

Where $\eta_{rs}(G)$ is the number of edges of G such that $pq \in E(G) \{ r_p , r_q \} = \{r, s\}$

Table 2: Derivation of topological Indices from M polynomial

S. No.	Topological index	Formula	Derivation from M Polynomial
1	First Zagreb index	$\sum_{e \in E(G)} (r_a + r_b)$	$(\delta_a + \delta_b) f(a, b)\|_{a=b=1}$
2	Second Zagreb index	$\sum_{e \in E(G)} (r_a r_b)$	$(\delta_a \delta_b) f(a, b)\|_{a=b=1}$
3	Forgotten index	$\sum_{e \in E(G)} (r_a{}^2 + r_b{}^2)$	$(\delta_a{}^2 + \delta_b{}^2) f(a, b)\|_{a=b=1}$
4	Harmonic Index	$\sum_{e \in E(G)} \frac{2}{(r_a + r_b)}$	$(2S_a J) f(a, b)\|_{a=b=1}$

Where

$\delta_a = a \left(\frac{\partial (f(a,b))}{\partial a}\right)$ ----------------------- (3.1)

$\delta_b = b \left(\frac{\partial (f(a,b))}{\partial b}\right)$ ----------------------- (3.2)

$s_a = \int_0^a \frac{f(r,b)}{r} dr$ ----------------------- (3.3)

Main results

In this section we obtain the expressions for *M-polynomials* of molecular graphs of famotidine using combinatorial computation degree counting method based on vertices and edges partition technique.

The molecular graph of famotidine having vertices V(F) = 20 and Edges E(F) =20

Theorem 3.1:

Let F be the graph of famotidine then the M polynomial of F is $M(F;a,b) = 3ab3ab^3 + 9a^2b^3 + 4a^2b^2 + 3ab^4 + a^2b^4$

Proof:

Consider the graph of famotidine. The edge partition of famotidine is

$$|E_{1,3}| = 3;\ |E_{2,2}| = 4\ ;|E_{2,3}| = 9;\ |E_{1,4}| = 3; |E_{2,4}| = 1$$

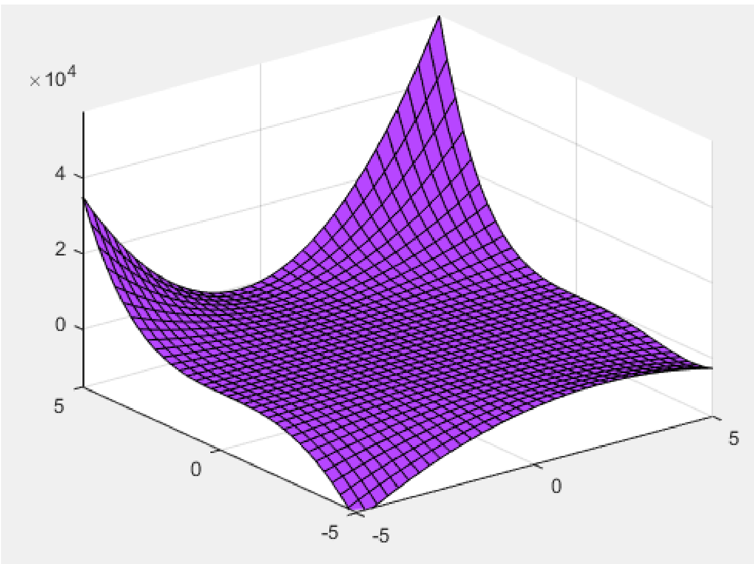
$$M(F;a,b) = \sum_{r\le s} \eta_{rs}(F)a^r b^s$$

$$M(F;a,b) = \sum_{1\le 3} \eta_{13}(F)a^1b^3 + \sum_{2\le 3} \eta_{23}(F)a^2b^3 + \sum_{2\le 2} \eta_{22}(F)a^2b^2 + \sum_{1\le 4} \eta_{14}(F)a^1b^4 + \sum_{2\le 4} \eta_{24}(F)a^2b^4$$

$$= |E_{1,3}|a^1b^3 + |E_{2,3}|\,a^2b^3 + |E_{2,2}|\,a^2b^2 + |E_{1,4}|a^1b^4 + |E_{2,4}|a^2b^4$$

$$= 3a^1b^3 + 9\,a^2b^3 + 4\,a^2b^2 + 3a^1b^4 + a^2b^4$$

$M(F;a,b)$ = $3ab^3 + 9\,a^2b^3 + 4\,a^2b^2 + 3ab^4 + a^2b^4$



Theorem 3.2:

Let F be the graph of famotidine then the M polynomial first and second Zagreb indices of famotidine are

$$(\delta_a + \delta_b)f(a,b) = 94$$
$$(\delta_a\delta_b)f(a,b) = 99$$

Proof :

We know that

The M polynomial first and second Zagreb indices of famotidine are

$$M_1(F;a,b) = (\delta_a + \delta_b)f(a,b)|_{a=b=1}$$

Therefore

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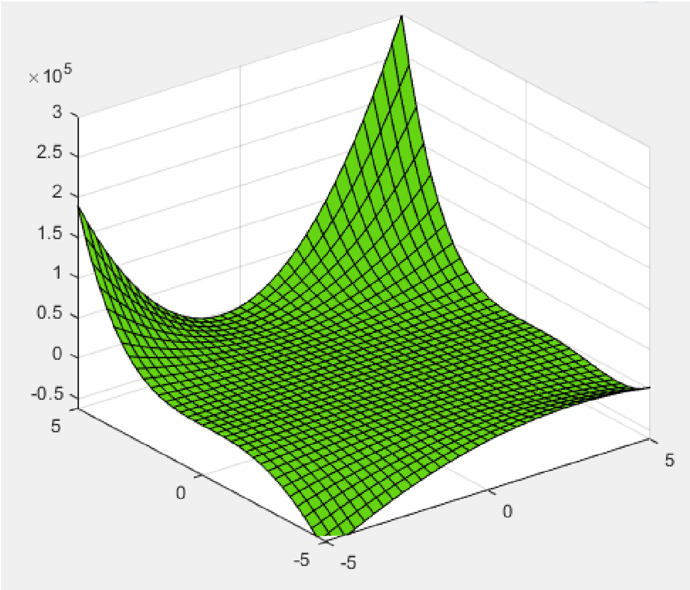
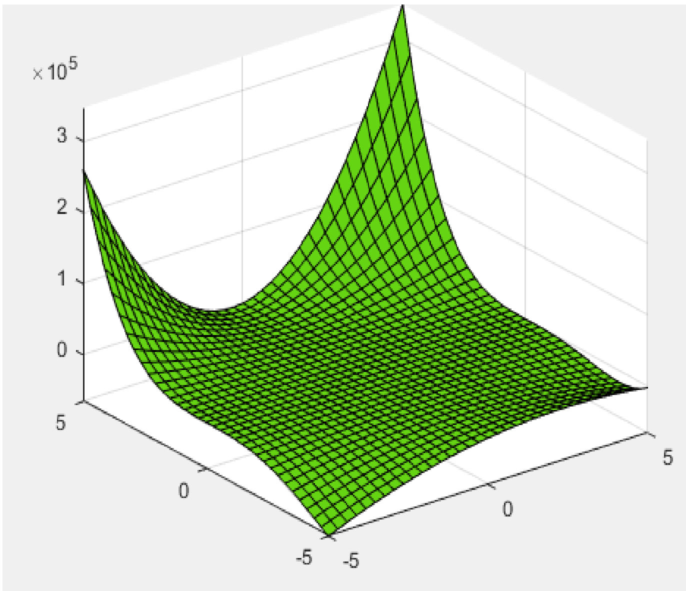
$$\delta_a f(a,b) = 3ab^3 + 18a^2b^3 + 8a^2b^2 + 3ab^4 + 2a^2b^4$$
$$\delta_b f(a,b) = 9ab^3 + 27a^2b^3 + 8a^2b^2 + 12ab^4 + 4a^2b^4$$
$$(\delta_a + \delta_b) f(a,b) = 12ab^3 + 45a^2b^3 + 16a^2b^2 + 15ab^4 + 6a^2b^4$$
$$(\delta_a + \delta_b) f(a,b)|_{a=b=1} = 94$$

Similarly,

$$M_2(F;a,b) = (\delta_a\delta_b) f(a,b)|_{a=b=1}$$
$$(\delta_a\delta_b) f(a,b)|_{a=b=1} = 99$$

Hence, $M[M_1F;a,b] = 94$ and $M[M_2F;a,b] = 99$





Theorem 3.3:
Let F be the molecular graph of famotidine then the M polynomial of forgotten index is 250.
Proof:
We know that,
The M polynomial of forgotten index is

$$(\delta_a^2 + \delta_b^2) f(a,b)|_{a=b=1}$$

Therefore,

$$\delta_a^2 f(a,b) = 3ab^3 + 36a^2b^3 + 16a^2b^2 + 3ab^4 + 4a^2b^4$$
$$\delta_b^2 f(a,b) = 27ab^3 + 81a^2b^3 + 16a^2b^2 + 48ab^4 + 16a^2b^4$$

$$(\delta_a^2 + \delta_b^2) f(a,b) = 30ab^3 + 117a^2b^3 + 32a^2b^2 + 51ab^4 + 20a^2b^4$$

$$(\delta_a^2 + \delta_b^2) f(a,b)|_{a=b=1} = 250$$

Hence, $M[FF;a,b]|_{a=b=1} = 250$

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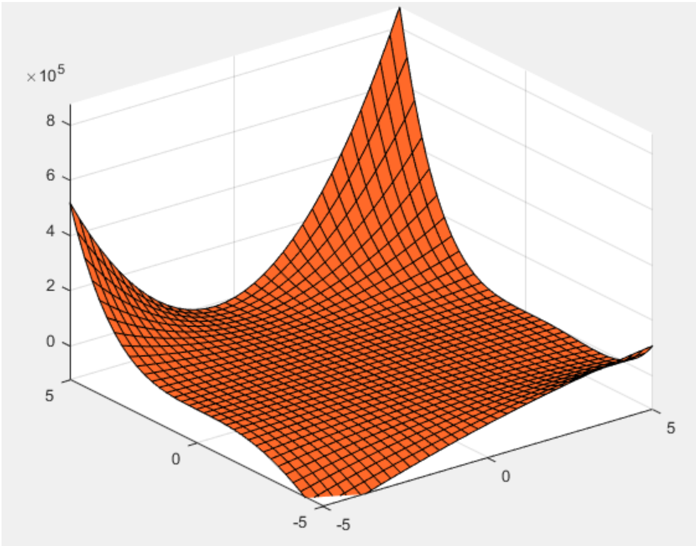
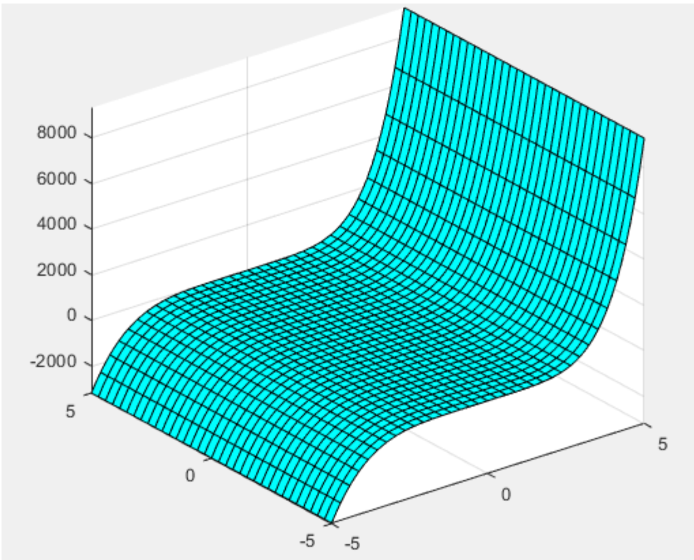


Theorem 3.4:
Let F be the famotidine graph, then the M polynomial of harmonic index is 7.1.
Proof:
We know that,
The M Polynomial of Harmonic Index is,

$$(2S_aJ)f(a,b)|_{a=b=1}$$

Now,
Using Equation 3.3 wee get, the required result is
$M[HF;a,b] = \ 2a^5 + \frac{7}{5}a^4 + \frac{1}{7}a^6$

$$M[HF;a,b]|_{a=b=1} = 7.1$$



Conclusion
The analysis of the characteristics of the molecular structure plays a crucial role in the progress of medical science. In the case of Famotidine, various topological indices of chemical graph theory, such as the first and second Zagreb indices, the first and second Zagreb eccentricity indices, the first and second location indices, Famotidine Sanskruti indices, and other topological indices, were calculated to determine the physical and chemical properties of the studied molecules. This research utilized the M polynomial to calculate these topological indices, including

the ABC index, ABC4 index, Randic connectivity index, combination index, GA index, GA5 index, first Zagreb index, second Zagreb index, integrated Zagreb index, harmonic index, and more.By understanding the topological symbols and properties of Famotidine, Researchers can further explore its potential applications and develop more effective treatments for acid reflux and heartburn.

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