

A Study of Neighborhood M-Polynomials of Gastrocolic Drugs Using Topological Indices

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1 Abstract:

Topological indices are the numerical values that are abundantly used in chemo metrics, bio medicines, and bio informatics for finding physico-chemical and biological activities with in molecular structure. This study is mainly focused on neighborhood M-Polynomial (NM-Polynomial) for calculating degree based topological indices. The topological index can be utilized to ascertain the chemical and biological qualities that are displayed. Compound physical properties and chemical reactivity can be better understood by utilizing a topological index, which is a numerical value that represents the full molecular graph structure. Our aim is to find degree based and neighborhood degree based indices for Omeprazole, Pantoprazole and Ranitidine by applying the innovative method of calculating NM-Polynomials we establish a fresh perspective on molecular structure and topological indices. Chemical graph theory is a branch of mathematical chemistry which has an important outcome on the development of the chemical science . **Key words:** Ranitidine, Pantoprazole, Omeprazole.

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2 Introduction:

Chemical graph theory is a branch of mathematical chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically. A molecular graph is a simple, finite graph in which vertices denote the atoms and edges denote the chemical bonds in chemical structure. Recently, researchers have turned their attention to designing topological indices based on the neighborhood degrees of vertex [1-7]. By the neighborhood degree of a node, we mean the totality of degree of all nodes that are connected to the node. The degree of a vertex is the total number of edges incident to the vertex. To make the neighborhood degree-based topological indices easier, present author introduced neighborhood M-Polynomials [8], whose role for neighborhood degree-based indices is parallel to polynomials for degree-based topological indices. Gastrointestinal problems are very common in all people around the world, which may be any condition or disorder that affects the stomach or gastrointestinal system, leading to symptoms such as vomiting or change in the bowl habit, abdominal pain, bloating, indigestion, and nausea. These problems can arise from various factors, including infection, inflammation, dietary choices, lifestyle factors, medications, or underlying medical conditions [9].

Omeprazole is a gastric acid proton-pump inhibitor that dose-dependently controls gastric acid secretion. The drug has greater anti-secretory activity than histamine H_2 receptor antagonists. Omeprazole is generally well tolerated during short (≤ 12 weeks) and long (up to 10 years and more) term treatment of peptic ulcer disease [10].

Pantoprazole is a potent and selective proton pump inhibitor. It is an effective agent in the treatment of peptic ulcers. Gastro-oesophageal reflux disease (GERD). Oesophagitis, Zollinger-Ellison syndrome, and other GI hypersecretory disorders have poor bioavailability and aqueous solubility; thus, its absorption and dissolution rate are limited, delaying its one set of actions.

Ranitidine is a histamine 2 blocker that decreases the amount of acid created by the stomach. Prescription ranitidine is approved for multiple indications, including the treatment and prevention of ulcers of the stomach and intestines and the treatment of gastroesophageal reflux disease. Ranitidine is used to treat ulcer gastroesophageal reflux disease (GERD), a condition in which backward flow of acid from the stomach causes heartburn and injury of the food pipe (esophagus), and conditions where the stomach produces too much acid, such as Zollinger-Ellison syndrome. Over the counter Ranitidine is used to prevent and treat symptoms of heartburn associated with acid indigestion and sour stomach. Ranitidine is in a class of medications called H_2 blockers. It decreases the amount of acid made in the stomach.[11] In 1878, James J. Sylvester (1814–1897) coined the term "graph". Currently one of the fields in graph theory with the quickest rate of growth is chemical

graph theory, which includes mathematical chemistry as a subfield. Ante Graovac, Milan Randić, Alexander Balaban, Haruo Hosoya, Nenad Trinajstić, and Ivan Gutman were the ones that invented [12,13,14]

Bollabas and Erdős created the broad Randić Index. The Harmonic index, which Fojilowicz, Gutman, and Trinajstić devised, supplanted the Randić index. In 1972, they discovered the first degree-based molecular descriptor which is currently referred to as the Zagreb index. Deutsch and Kalzior [15,16] created the M-Polynomial one of the new tools that have become available to all [17,18] which was introduced by Mondal et al [19, 20, 21], NM-polynomials are critical for starting closed methods of various degree based topological indices. Recently several researchers have focused on neighborhood degree based indices, which was increased interest for researchers on NM-Polynomials, These polynomials are very useful in determining neighborhood degree sum based graphical indices [22,23].

All molecular graphs in this article are finite, connected without loops and multiple edges. Let $G = (V, E)$ be a graph with vertex set as V and edge set as E . The degree of the vertices $u \in V(G)$ is denoted by d_u and is the number of vertices that are adjacent to u . The edge connecting the vertices u and v is denoted by $e = uv$ [24].

3 Preliminaries:

Let R be a simple connected graph and NM-polynomial can be represented by the following equations:

$$NM(G, R, S) = \sum_{i \leq j} R_{ij}(G) x^i x^j$$

$R_{i,j}$ denotes the number of edges $u, v \in E(G)$ where $nd_u, nd_v = i, j$, respectively in which nd_u, nd_v denotes the degrees of the vertices u and v respectively. For neighborhood degree-based TIs .

$\delta_u = nd_u, \delta_v = nd_v$, $NM(R : x, y) = f(x, y)$ the degree-based and neighborhood-degree-based TIs for the graph R are tabulated in Table 1. [25]

molecular descriptors and $NM(G)$ expressions

molecular descriptors	Mathematical expressions	Derivation from $NM(G, x, y)$
First Neighborhood Zagreb Index	$M_1(G) = \sum_{u,v \in E(G)} (d_u + d_v)$	$(D_x + D_y)(NM(G, x, y)) _{x=y=1}$
Neighborhood second Zagreb index	$M_2(G) = \sum_{u,v \in E(G)} (d_u \cdot d_v)$	$(D_x \cdot D_y)(NM(G, x, y)) _{x=y=1}$
Neighborhood Third Zagreb index	$M_3(G) = \sum_{u,v \in E(G)} (d_u^2 + d_v^2)$	$(D_x^2 + D_y^2)(NM(G, x, y)) _{x=y=1}$
Third NDe	$NDe_3(G) = \sum_{u,v \in E(G)} (d_u \cdot d_v)(d_u + d_v)$	$(D_x D_y)(D_x + D_y)(NM(G, x, y)) _{x=y=1}$
Fifth NDe	$NDe_5 = \sum_{u,v \in E(G)} (d_u^2 + d_v^2)$	$(D_x S_y + S_x D_y)(NM(G, x, y)) _{x=y=1}$
Neighborhood inverse sum indeg index	$ISI(G) = \sum_{u,v \in E(G)} \left(\frac{d_u d_v}{d_u + d_v} \right)$	$S_x J(D_x D_y)(NM(G, x, y)) _{x=y=1}$
Neighborhood Harmonic Index	$NH(G) = \sum_{u,v \in E(G)} \frac{2}{d_u + d_v}$	$2S_x J(NM(G, x, y)) _{x=y=1}$

$$D_x = x \left(\frac{\delta(f(x, y))}{\delta x} \right), D_y = y \left(\frac{\delta(f(x, y))}{\delta y} \right), J(f(x, y)) = f(x, y)|_{x=y=1},$$

$$S_x = \int_0^x \frac{f(x, y)}{t} dt|_{x=y=1}, S_y = \int_0^y \frac{f(x, y)}{t} dt|_{x=y=1}$$

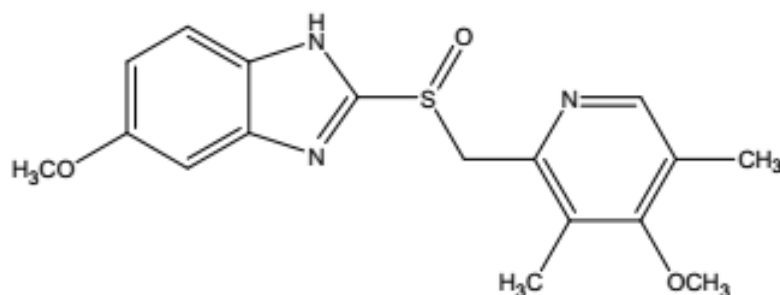


Figure 1: Omeprazole

4 Results:

With respect to the edge partition the work deals with neighborhood degree sum-based indices for Omeprazole, Pantoprazole and Ranitidine. We calculated NM-Polynomials by using various degree based topological indices

Number of edges	(2,4)	(4,6)	(6,6)	(6,5)	(5,5)	(5,7)	(7,7)	(7,8)	(2,7)	(8,6)	(8,7)	(5,6)	(3,7)	(6,3)
Frequency	2	1	3	5	3	4	1	1	1	1	1	4	1	1

Theorem 1:

The NM-Polynomial of Omeprazole

$$2x^2y^4 + x^4y^6 + 3x^6y^6 + 5x^6y^5 + 5x^5y^5 + 4x^5y^7 + x^7y^8 + x^2y^7 + x^8y^6 + 4x^5y^6 + x^3y^7 + x^6y^3$$

Proof: From fig. 1, we can see that the edge set of Omeprazole has 25 edges.

$$NE_{(2,4)} = [e = uv \in E(G) | d_u = 2, d_v = 4]$$

$$NE_{(4,6)} = [e = uv \in E(G) | d_u = 4, d_v = 6]$$

$$NE_{(6,6)} = [e = uv \in E(G) | d_u = 6, d_v = 6]$$

$$NE_{(6,5)} = [e = uv \in E(G) | d_u = 6, d_v = 5]$$

$$NE_{(5,5)} = [e = uv \in E(G) | d_u = 5, d_v = 5]$$

$$NE_{(5,7)} = [e = uv \in E(G) | d_u = 5, d_v = 7]$$

$$NE_{(7,7)} = [e = uv \in E(G) | d_u = 7, d_v = 7]$$

$$NE_{(7,8)} = [e = uv \in E(G) | d_u = 7, d_v = 8]$$

$$NE_{(2,7)} = [e = uv \in E(G) | d_u = 2, d_v = 7]$$

$$NE_{(8,6)} = [e = uv \in E(G) | d_u = 8, d_v = 6]$$

$$NE_{(8,7)} = [e = uv \in E(G) | d_u = 8, d_v = 7]$$

$$NE_{(5,6)} = [e = uv \in E(G) | d_u = 5, d_v = 6]$$

$$NE_{(3,7)} = [e = uv \in E(G) | d_u = 3, d_v = 7]$$

$$NE_{(6,3)} = [e = uv \in E(G) | d_u = 6, d_v = 3]$$

Such that

$$\begin{aligned} |NE_{(2,4)}| &= 2, |E_{(4,6)}| = 1, |NE_{(6,6)}| = 3, |E_{(6,5)}| = 5, |NE_{(5,5)}| = 3, \\ |E_{(5,7)}| &= 4, |NE_{(7,7)}| = 1, |E_{(7,8)}| = 1, |NE_{(2,7)}| = 1, |E_{(8,6)}| = 1, \\ |NE_{(8,7)}| &= 1, |E_{(5,6)}| = 4, |NE_{(3,7)}| = 1, |E_{(6,3)}| = 1 \end{aligned}$$

$$NM(G, R, S) = \sum_{i \leq j} R_{ij}(G) x^i x^j$$

$$= \sum_{2 \leq 4} R_{2,4}(G) x^2 x^4 + \sum_{4 \leq 6} R_{4,6}(G) x^4 x^6$$

+

$$\sum_{6 \leq 6} R_{6,6}(G) x^6 x^6 + \sum_{6 \leq 5} R_{6,5}(G) x^6 x^5$$

+

$$\sum_{5 \leq 5} R_{5,5}(G) x^5 x^5 + \sum_{5 \leq 7} R_{5,7}(G) x^5 x^7$$

+

$$\sum_{7 \leq 7} R_{7,7}(G) x^7 x^7 + \sum_{7 \leq 8} R_{7,8}(G) x^7 x^8$$

+

$$\sum_{8 \leq 7} R_{2,7}(G) x^2 x^7 + \sum_{8 \leq 7} R_{8,7}(G) x^8 x^7$$

+

$$\sum_{8 \leq 6} R_{8,6}(G) x^8 x^6 + \sum_{5 \leq 6} R_{5,6}(G) x^5 x^6$$

+

$$\sum_{3 \leq 7} R_{3,7}(G) x^3 x^7 + \sum_{6 \leq 3} R_{6,3}(G) x^6 x^3$$

$$= 2x^2y^4 + x^4y^6 + 3x^6y^6 + 5x^6y^5 + 5x^5y^5$$

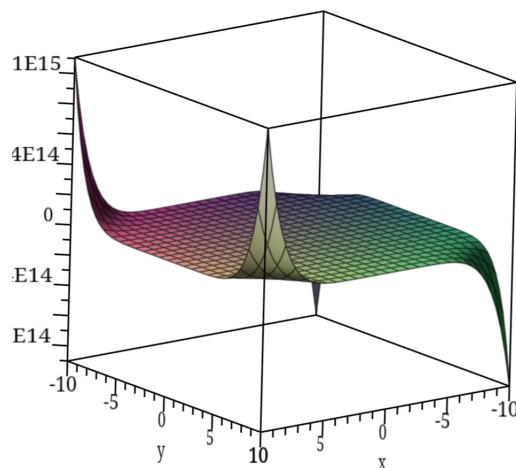


Figure 2: The 3D plot of NM-Polynomial of Omeprazole

$$+4x^5y^7 + x^7y^8 + x^2y^7 + x^8y^6 + 4x^5y^6 + x^3y^7 + x^6y^3$$

Corollary 1: Let G be a graph of Omeprazole, then we have the following connectivity-dependent topological indices:

$$1. NM_1(G, x, y) = (D_x + D_y)F(x, y)_{x=y=1} = 310$$

$$2. NM_2(G, x, y) = (D_x \cdot D_y)F(x, y)_{x=y=1} = 839$$

$$3. NM_3(G, x, y) = (D_x^2 + D_y^2)F(x, y)_{x=y=1} = 1700$$

$$4.NM(G, x, y) = (D_x D_y)(D_x + D_y)F(x, y)_{x=y=1} = 9848$$

$$5.NM(G, x, y) = (D_x S_y + S_x D_y)F(x, y)_{x=y=1} = 54.893$$

$$6.NM(G, x, y) = 2(S_x J)F(x, y)_{x=y=1} = 12.3881$$

$$7.NM(G, x, y) = (S_x J D_x D_y)F(x, y)_{x=y=1} = 74.6962$$

Proof:The following calculations are done by using the above formula:

$$D_x(NM(G, R, S)) = 4x^2y^4 + 4x^4y^6 + 18x^6y^6 + 30x^6y^5 + 15x^5y^5$$

$$+ 20x^5y^7 + 7x^7y^8 + 2x^2y^7 + 8x^8y^6 + 20x^5y^6 + 3x^3y^7 + 6x^6y^3$$

$$D_y(NM(G, R, S)) = 8x^2y^4 + 6x^4y^6 + 18x^6y^6 + 25x^6y^5 + 15x^5y^5$$

$$+ 28x^5y^7 + 7x^7y^7 + 8x^7y^8 + 7x^2y^7 + 6x^8y^6 + 24x^5y^6 + 7x^3y^7 + 3x^6y^3$$

$$S_x = \int_0^x \frac{F(x, y)}{t} \Big|_{x=t} dt = x^2y^4 + \frac{x^4y^6}{4} + \frac{x^6y^6}{2} + \frac{5x^6y^5}{6} + \frac{3x^5y^5}{5} + \frac{4x^5y^7}{7}$$

$$+ \frac{x^7y^7}{7} + \frac{x^7y^8}{7} + \frac{x^2y^7}{2} + \frac{x^8y^6}{8} + \frac{4x^5y^6}{5} + \frac{x^3y^7}{3} + \frac{x^6y^3}{6}$$

$$S_y = \int_0^y \frac{F(x, y)}{t} \Big|_{y=t} dt = \frac{x^2y^4}{2} + \frac{x^4y^6}{6} + \frac{x^6y^6}{2} + x^6y^5 + \frac{3x^5y^5}{5} + \frac{4x^5y^7}{7}$$

$$+ \frac{x^7y^7}{7} + \frac{x^7y^8}{8} + \frac{x^2y^7}{7} + \frac{x^8y^6}{6} + \frac{4x^5y^6}{6} + \frac{x^3y^7}{7} + \frac{x^6y^3}{3}$$

$$NM_1(G, x, y) = (D_x + D_y)F(x, y)_{x=y=1}$$

$$= 12x^2y^4 + 10x^4y^6 + 36x^6y^6 + 55x^6y^5 + 30x^5y^5 + 48x^5y^7 + 14x^7y^6$$

$$+ 15x^7y^8 + 9x^2y^7 + 14x^8y^6 + 48x^5y^6 + 10x^3y^7 + 9x^6y^3$$

$$= 310$$

$$NM_2(G, x, y) = (D_x \cdot D_y)F(x, y)_{x=y=1}$$

$$= 16x^2y^4 + 24x^2y^6 + 108x^6y^6 + 150x^6y^5 + 75x^5y^5 + 140x^5y^7 + 49x^7y^7$$

$$+ 56x^7y^8 + 14x^2y^7 + 48x^8y^6 + 120x^5y^6 + 21x^3y^7 + 18x^6y^3$$

$$839$$

$$NM_3(G, x, y) = (D_x^2 + D_y^2)F(x, y)_{x=y=1}$$

$$= 40x^2y^4 + 52x^4y^6 + 216x^6y^6 + 200x^5y^5 + 175x^5y^5 + 296x^5y^7 + 98x^7y^7$$

$$+ 113x^7y^8 + 53x^2y^7 + 100x^8y^6 + 244x^5y^6 + 58x^3y^7 + 55x^6y^3$$

$$= 1700$$

$$NM(G, x, y) = (D_x D_y)(D_x + D_y)F(x, y)_{x=y=1}$$

$$\begin{aligned}
&= 96x^2y^4 + 240x^4y^6 + 1296x^6y^6 + 1650x^6y^5 + 750x^5y^5 + 1680x^5y^7 \\
&+ 686x^5y^7 + 840x^7y^8 + 126x^2y^7 + 672x^8y^6 + 1440x^5y^6 + 210x^3y^7 + 162x^6y^3
\end{aligned}$$

$$9848$$

$$NM(G, x, y) = (D_x S_y + S_x D_y) F(x, y)_{x=y=1}$$

$$S_x D_y = 4x^2y^4 + \frac{3x^4y^6}{2} + 3x^6y^6 + \frac{25x^6y^5}{6} + \frac{3x^5y^5}{5} + \frac{28x^5y^5}{5}$$

$$+ x^7y^7 + \frac{8x^7y^8}{7} + \frac{7x^2y^7}{2} + \frac{3x^8y^6}{4} + \frac{24x^5y^6}{5} + \frac{7x^3y^7}{3} + \frac{x^6y}{2}$$

$$= 54.893$$

$$D_x S_x = 2x^2y^4 + x^4y^6 + x^6y^6 + 5x^6y^5 + 3x^5y^5 + x^7y^7 + x^7y^8$$

$$+ x^2y^7 + x^8y^6 + 4x^5y^6 + x^3y^7 + x^6y^3$$

$$= 22$$

$$(D_x S_y + S_x D_y) F(x, y)_{x=y=1} = 54.893$$

$$NM(G, x, y) = 2(S_x J) F(x, y)_{x=y=1}$$

$$12.3881$$

$$9$$

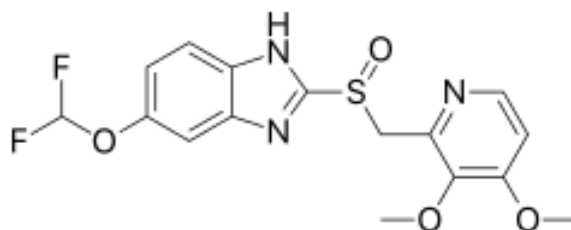


Figure 3: Pantoprazole

$$\begin{aligned}
 NM(G, x, y) &= (S_x J D_x D_y) F(x, y)_{x=y=1} \\
 &= \frac{8x^6}{3} + 3x^8 + 9x^{12} + \frac{150x^{11}}{11} + \frac{75x^{10}}{10} + \frac{35x^{12}}{3} \\
 &\quad + \frac{7x^{14}}{2} + \frac{56x^{15}}{15} + \frac{14x^9}{9} + \frac{24x^{14}}{7} + \frac{120x^{11}}{11} + \frac{21x^{10}}{10} + 2x^9 \\
 &= 74.6962
 \end{aligned}$$

5 NM Polynomials of Pantoprazole

Number of edges	(3,4)	(4,6)	(6,6)	(5,5)	(6,7)	(5,7)	(7,7)	(4,2)	(4,8)	(8,7)	(5,4)	(7,4)
Frequency	2	1	4	2	1	3	1	2	1	2	2	1

Theorem 2: The NM-Polynomial of Pantoprazole

$$2x^3y^4 + 3x^5y^7 + 2x^5y^4 + x^4y^4 + x^4y^6 + x^7y^7 + x^7y^4 + 4x^6y^6 + 2x^4y^2 + 2x^5y^5 + x^4y^8 + x^6y^7 + 2x^8y^7$$

Proof: From Fig. 2, we can see that the edge set of Pantoprazole has 27 edges.

$$NE_{(3,4)} = [e = uv \in E(G) | d_u = 3, d_v = 4]$$

$$NE_{(4,6)} = [e = uv \in E(G) | d_u = 4, d_v = 6]$$

$$NE_{(6,6)} = [e = uv \in E(G) | d_u = 6, d_v = 6]$$

$$NE_{(5,5)} = [e = uv \in E(G) | d_u = 6, d_v = 5]$$

$$NE_{(6,7)} = [e = uv \in E(G) | d_u = 6, d_v = 7]$$

$$NE_{(5,7)} = [e = uv \in E(G) | d_u = 5, d_v = 7]$$

$$NE_{(7,7)} = [e = uv \in E(G) | d_u = 7, d_v = 7]$$

$$NE_{(4,2)} = [e = uv \in E(G) | d_u = 4, d_v = 2]$$

$$NE_{(4,8)} = [e = uv \in E(G) | d_u = 4, d_v = 8]$$

$$NE_{(8,7)} = [e = uv \in E(G) | d_u = 8, d_v = 7]$$

$$NE_{(5,4)} = [e = uv \in E(G) | d_u = 5, d_v = 4]$$

$$NE_{(7,4)} = [e = uv \in E(G) | d_u = 7, d_v = 4]$$

Such that

$$\begin{aligned} |NE_{(2,4)}| &= 2, |E_{(4,6)}| = 1, |NE_{(6,6)}| = 4, |E_{(5,5)}| = 2, |NE_{(6,7)}| = 1, \\ |E_{(5,7)}| &= 3, |NE_{(7,7)}| = 1, |E_{(4,2)}| = 2, |NE_{(4,8)}| = 1, |E_{(8,7)}| = 2, \\ |NE_{(5,4)}| &= 2, |E_{(7,4)}| = 1 \end{aligned}$$

$$NM(G, R, S) = \sum_{i \leq j} R_{ij}(G) x^i x^j$$

$$= R_{3,4} x^3 y^4 + R_{5,7} x^5 y^7 + R_{5,4} x^5 y^4 + R_{4,6} x^4 y^6 + R_{7,7} x^7 y^7 +$$

$$+ R_{7,4} x^7 y^4 + R_{6,6} x^6 y^6 + R_{4,2} x^4 y^2 + R_{5,5} x^5 y^5 + R_{4,8} x^4 y^8 + R_{6,7} x^6 y^7 + R_{8,7} x^8 y^7$$

$$= 2x^3 y^4 + 3x^5 y^7 + 2x^5 y^4 + x^4 y^4 + x^4 y^6 + x^7 y^7 + x^7 y^4 + 4x^6 y^6 +$$

$$2x^4 y^2 + 2x^5 y^5 + x^4 y^8 + x^6 y^7 + 2x^8 y^7$$

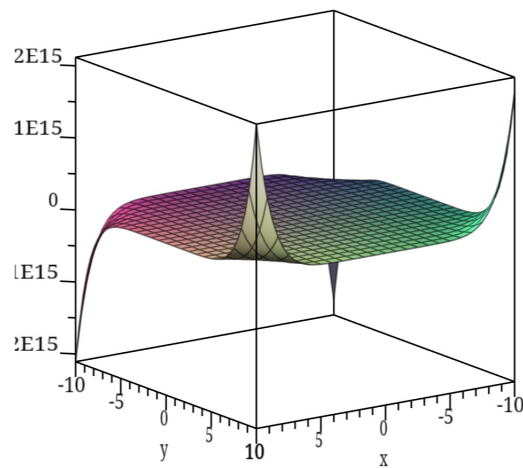


Figure 4: The 3D plot of NM-Polynomial of Pantoprazole

$$D_x(NM(G, R, S)) = 6x^3y^4 + 15x^5y^7 + 10x^5y^4 + 4x^4y^6 + 7x^7y^7 + 7x^7y^4 \\ + 24x^6y^6 + 8x^4y^2 + 10x^5y^5 + 4x^4y^8 + 6x^6y^7 + 16x^8y^7$$

Corollary 2: Let G be a graph of Pantoprazole, Then we have the following connectivity-dependent topological indices:

$$1. NM_1(G, x, y) = (D_x + D_y)F(x, y)|_{x=y=1} = 238$$

$$2. NM_2(G, x, y) = (D_x \cdot D_y)F(x, y)|_{x=y=1} = 666$$

$$3.NM_3(G, x, y) = (D_x^2 + D_y^2)(F(x, y)|_{x=y=1} = 1388$$

$$4.NM(G, x, y) = (D_x D_y)(D_x + D_y)F(x, y)|_{x=y=1} = 7824$$

$$5.NM(G, x, y) = (D_x S_y + S_x D_y)F(x, y)|_{x=y=1} = 45.157$$

$$6.NM(G, x, y) = 2(S_x J)F(x, y)|_{x=y=1} = 7.182$$

$$7.NM(G, x, y) = S_x J D_x D_y F(x, y)|_{x=y=1} = 57.654$$

Proof:The following calculations are done by using the above formula:

$$D_y(NM(G, R, S)) = 8x^3y^4 + 21x^5y^7 + 8x^5y^4 + 6x^4y^6 + 7x^7y^7 + 4x^7y^4$$

$$+ 24x^6y^6 + 4x^4y^2 + 10x^5y^5 + 8x^4y^8 + 7x^6y^7 + 14x^8y^7$$

$$S_x = \int_0^x \frac{F(x, y)}{t} \Big|_{x=t} dt$$

$$= \frac{2x^3y^4}{3} + \frac{3x^5y^7}{5} + \frac{2x^5y^4}{5} + \frac{x^4y^6}{4} + \frac{x^7y^7}{7}$$

$$+ \frac{x^7y^4}{7} + \frac{4x^6y^6}{6} + \frac{2x^4y^2}{4} + \frac{2x^5y^5}{5} + \frac{x^4y^8}{4} + \frac{x^6y^7}{6} + \frac{2x^8y^7}{8}$$

$$S_y = \int_0^y \frac{F(x, y)}{t} \Big|_{y=t} dt$$

$$= \frac{x^3y^4}{2} + \frac{3x^5y^7}{7} + \frac{x^5y^4}{2} + \frac{x^4y^6}{6} + \frac{x^7y^7}{7}$$

$$+ \frac{x^7y^4}{4} + \frac{2x^6y^6}{3} + \frac{x^4y^2}{1} + \frac{2x^5y^5}{5} + \frac{x^4y^8}{8} + \frac{x^6y^7}{7} + \frac{2x^8y^7}{7}$$

$$NM_1(G, x, y) = (D_x + D_y)F(x, y)|_{x=y=1}$$

$$= 14x^3y^4 + 36x^5y^7 + 18x^5y^4 + 10x^4y^6 + 14x^7y^7 + 11y^7x^4 + 48x^6y^6$$

$$+ 12x^4y^2 + 20x^5y^5 + 12x^4y^8 + 13x^6y^7 + 30x^8y^7$$

$$= 238$$

$$NM_2(G, x, y) = (D_x \cdot D_y)F(x, y)|_{x=y=1}$$

$$= 24x^3y^4 + 105x^5y^7 + 40x^5y^4 + 24x^4y^6 + 49x^7y^7 + 28y^7x^4 + 144x^6y^6$$

$$+ 16x^4y^2 + 50x^5y^5 + 32x^4y^8 + 42x^6y^7 + 112x^8y^7$$

$$= 666$$

$$NM_3(G, x, y) = (D_x^2 + D_y^2)(F(x, y)|_{x=y=1})$$

$$= 50x^3y^4 + 222x^5y^7 + 82x^5y^4 + 52x^4y^6 + 98x^7y^7 + 65x^7y^4 + 288x^6y^6$$

$$+ 40x^4y^2 + 100x^5y^5 + 80x^4y^8 + 85x^6y^7 + 226x^8y^7$$

$$= 1388$$

$$\begin{aligned}
NM(G, x, y) &= (D_x D_y)(D_x + D_y)F(x, y)|_{x=y=1} \\
&= 168x^3y^4 + 1260x^5y^2 + 360x^5y^4 + 240x^4y^6 + 686x^7y^7 + 176y^7x^4 \\
&\quad + 1728x^6y^6 + 96x^4y^2 + 500x^5y^7 + 384x^4y^8 + 546x^6y^7 + 1680x^8y^7
\end{aligned}$$

$$= 7824$$

$$\begin{aligned}
NM(G, x, y) &= (D_x S_y + S_x D_y)F(x, y)|_{x=y=1} \\
&= \frac{25x^3y^4}{6} + \frac{222x^5y^7}{35} + \frac{41x^5y^4}{10} + \frac{13x^4y^6}{6} + 2x^7y^7 + \frac{65x^7y^4}{28} \\
&\quad + 8x^6y^6 + 5x^4y^2 + 4x^5y^5 + \frac{5x^4y^8}{2} + \frac{85x^6y^7}{42} + \frac{71x^8y^7}{28}
\end{aligned}$$

$$45.157$$

$$\begin{aligned}
NM(G, x, y) &= 2(S_x J)F(x, y)|_{x=y=1} \\
&= \frac{4x^7}{3} + \frac{17x^{12}}{10} + \frac{4x^9}{9} + \frac{2x^{14}}{7} + \frac{13x^{10}}{10} + \frac{2x^{11}}{7} + x^6 + \frac{x^{13}}{3} + \frac{x^{15}}{2}
\end{aligned}$$

$$7.182$$

$$\begin{aligned}
NM(G, x, y) &= S_x J D_x D_y F(x, y)|_{x=y=1} \\
&= \frac{24x^7}{7} + \frac{105x^{12}}{12} + 4x^{10} + \frac{24x^{10}}{10} + \frac{7x^{14}}{2} + \frac{28x^{11}}{11} \\
&\quad + 12x^{12} + \frac{8x^6}{3} + 5x^{10} + \frac{8x^{12}}{3} + \frac{42x^{13}}{13} + \frac{112x^{15}}{15}
\end{aligned}$$

$$15$$

$$= 57.654$$

6 Results of Ranitidine:

Number of edges	(2,3)	(2,6)	(2,4)	(4,7)	(7,5)	(5,4)	(5,5)	(4,4)	(5,6)	(4,6)	(3,4)	(6,6)	(3,3)
Frequency	2	1	1	1	1	2	1	2	4	2	1	4	4

Theorem 3: The NM-Polynomial of Ranitidine

$$2x^2y^3 + x^2y^6 + x^2y^4 + x^4y^7 + x^7y^5 + 2x^5y^4 + x^5y^5 + 2x^4y^4 + 4x^5y^6 + 2x^4y^6 + x^3y^4 + 4x^6y^6 + 4x^3y^3$$

Proof: From Fig. 3, we can see that the edge set of Ranitidine has 21 edges.

$$NE_{(2,3)} = [e = uv \in E(G) | d_u = 2, d_v = 3]$$

$$NE_{(2,6)} = [e = uv \in E(G) | d_u = 2, d_v = 6]$$

$$NE_{(2,4)} = [e = uv \in E(G) | d_u = 2, d_v = 4]$$

$$NE_{(4,7)} = [e = uv \in E(G) | d_u = 4, d_v = 7]$$

$$NE_{(7,5)} = [e = uv \in E(G) | d_u = 7, d_v = 5]$$

$$NE_{(5,4)} = [e = uv \in E(G) | d_u = 5, d_v = 4]$$

$$NE_{(5,5)} = [e = uv \in E(G) | d_u = 5, d_v = 5]$$

$$NE_{(4,4)} = [e = uv \in E(G) | d_u = 4, d_v = 4]$$

$$NE_{(5,6)} = [e = uv \in E(G) | d_u = 5, d_v = 6]$$

$$NE_{(4,6)} = [e = uv \in E(G) | d_u = 4, d_v = 6]$$

$$NE_{(3,4)} = [e = uv \in E(G) | d_u = 3, d_v = 4]$$

$$NE_{(6,6)} = [e = uv \in E(G) | d_u = 6, d_v = 6]$$

$$NE_{(3,3)} = [e = uv \in E(G) | d_u = 3, d_v = 3]$$

Such that

$$\begin{aligned} |NE_{(2,3)}| &= 2, |E_{(2,6)}| = 1, |NE_{(2,4)}| = 1, |E_{(4,7)}| = 1, |NE_{(7,5)}| = 1, \\ |E_{(5,4)}| &= 2, |NE_{(5,5)}| = 1, |E_{(4,4)}| = 2, |NE_{(5,6)}| = 4, |E_{(4,6)}| = 2, |NE_{(3,4)}| = \\ 1, |NE_{(6,6)}| &= 4, |E_{(3,3)}| = 4 \end{aligned}$$

$$\begin{aligned} NM(G, R, S) &= \sum_{i \leq j} R_{ij}(G) x^i y^j \\ &= R_{2,3} x^2 y^3 + R_{2,6} x^2 y^6 + R_{2,4} x^2 y^4 + R_{4,7} x^4 y^7 + R_{5,4} x^5 y^4 \end{aligned}$$

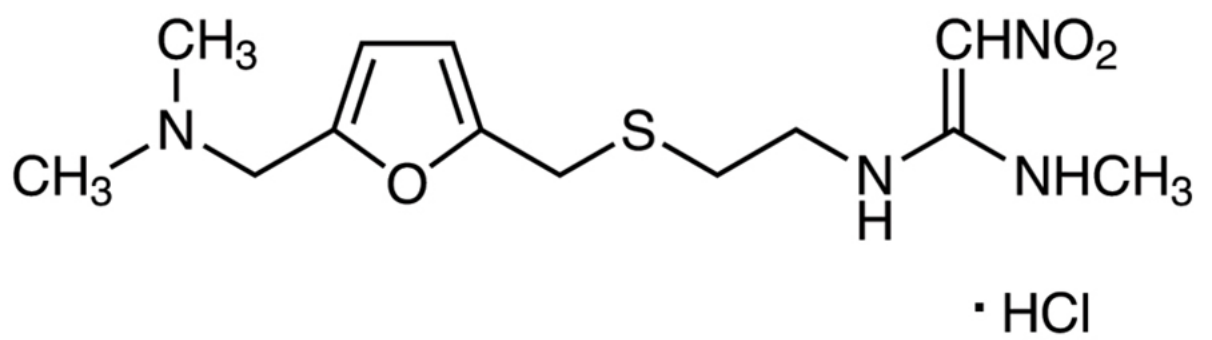


Figure 5: Ranitidine

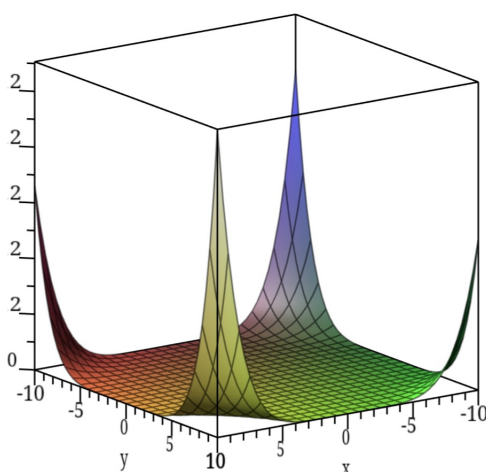


Figure 6: The 3D Plot of NM-Polynomial of Ranitidine

$$\begin{aligned}
 &+R_{5,5}x^5y^5+R_{4,4}x^4y^4+R_{5,6}x^5y^6+R_{4,6}x^4y^6+R_{3,4}x^3y^4+R_{6,6}x^6y^6+R_{3,3}x^3y^3 \\
 &= 2x^2y^3+x^2y^6+x^2y^4+x^4y^7+x^7y^5+2x^5y^4+x^5y^5+2x^4y^4+4x^5y^6+2x^4y^6+x^3y^4+4x^6y^6+4x^3y^3
 \end{aligned}$$

Corollary 3: Let G be a graph of Ranitidine. The following connectivity-dependent topological indices are available to us:

$$1.NM_1(G, x, y) = (D_x + D_y)F(x, y)|_{x=y=1} = 224$$

$$2.NM_2(G, x, y) = (D_x.D_y)F(x, y)|_{x=y=1} = 552$$

$$3.NM_3(G, x, y) = (D_x^2 + D_y^2)F(x, y)|_{x=y=1} = 5626$$

$$4.NM(G, x, y) = (D_xS_y + S_xD_y)F(x, y)|_{x=y=1} = 52.929$$

$$5.S_xJD_xD_y)F(x, y)|_{x=y=1}67.972$$

$$D_x(Nm(G, R, S)) = 4x^2y^3 + 2x^2y^6 + 2x^2y^4 + 4x^4y^7 + 7x^7y^5 + 10x^5y^4 + 5x^5y^5$$

$$+ 8x^4y^4 + 20x^5y^6 + 8x^4y^6 + 3x^3y^4 + 24x^6y^6 + 12x^3y^3$$

$$D_y(NM(G, R, S)) = 6x^2y^3 + 6x^2y^6 + 4x^2y^4 + 7x^4y^7 + 5x^7y^5 + 8x^5y^4$$

$$+ 5x^5y^5 + 8x^4y^4 + 24x^5y^6 + 12x^4y^6 + 4x^3y^4 + 24x^6y^6 + 12x^3y^3$$

$$S_x = \int_0^x \frac{F(x, y)}{t} \Big|_{x=t} dt = x^2y^3 + \frac{x^2y^6}{2} + \frac{x^2y^4}{2} + \frac{x^4y^7}{4} + \frac{x^7y^5}{7} + \frac{2x^5y^4}{5}$$

$$+ \frac{x^5y^5}{5} + \frac{x^4y^4}{2} + \frac{4x^5y^6}{5} + \frac{x^4y^6}{2} + \frac{x^3y^4}{3} + \frac{2x^6y^6}{3} + \frac{4x^3y^3}{3}$$

$$S_y = \int_0^y \frac{F(x, y)}{t} \Big|_{x=t} dt = \frac{2x^2y^3}{3} + \frac{x^2y^6}{6} + \frac{x^2y^4}{4} + \frac{x^4y^7}{7} + \frac{x^7y^5}{5} + \frac{2x^5y^4}{4}$$

$$+ \frac{x^5y^5}{5} + \frac{x^4y^4}{2} + \frac{2x^5y^6}{3} + \frac{x^4y^6}{3} + \frac{x^3y^4}{4} + \frac{2x^6y^6}{3} + \frac{4x^3y^3}{3}$$

$$NM_1(G, x, y) = (D_x + D_y)F(x, y)|_{x=y=1}$$

$$= 10x^2y^3 + 8x^2y^6 + 6x^2y^4 + 11x^4y^7 + 12x^7y^5 + 18x^5y^5 + 16x^4y^4$$

$$+ 44x^5y^6 + 20x^4y^6 + 7x^3y^4 + 48x^6y^6 + 24x^3y^3$$

$$= 224$$

$$NM_2(G, x, y) = (D_x \cdot D_y)F(x, y)|_{x=y=1}$$

$$= 12x^2y^3 + 12x^2y^6 + 8x^2y^4 + 28x^4y^7 + 35x^7y^5 + 40x^5y^4 + 25x^5y^5$$

$$+ 32x^4y^4 + 120x^5y^6 + 48x^4y^6 + 12x^3y^4 + 144x^6y^6 + 36x^3y^3$$

$$= 552$$

$$NM_3(G, x, y) = (Dx^2 + D_y^2)F(x, y)|_{x=y=1}$$

$$= 60x^2y^3 + 96x^2y^6 + 48x^2y^4 + 308x^4y^7 + 420x^7y^5 + 360x^5y^4 + 250x^5y^5$$

$$+ 256x^4y^4 + 1320x^5y^6 + 480x^4y^6 + 84x^3y^4 + 1728x^6y^6 + 216x^3y^3$$

$$= 5,626$$

$$NM(G, x, y) = (D_x S_y + S_x D_y)F(x, y)|_{x=y=1}$$

$$= \frac{13x^2y^3}{3} + \frac{10x^2y^6}{3} + \frac{7x^3y^4}{6} + \frac{65x^4y^7}{28} + \frac{74x^7y^7}{35} + \frac{41x^5y^4}{10}$$

$$+ 2x^5y^5 + 4x^4y^4 + \frac{122x^5y^6}{15} + \frac{13x^4y^6}{3} + \frac{25x^5y^4}{12} + 7x^6y^6 + 8x^3y^3$$

$$= 52.929$$

$$S_x J D_x D_y)F(x, y)|_{x=y=1}$$

$$= \frac{12x^5}{5} + \frac{3x^8}{2} + \frac{4x^6}{3} + \frac{28x^{11}}{11} + \frac{35x^{12}}{12} + \frac{40x^9}{9} +$$

$$\frac{25x^{10}}{10} + 4x^8 + \frac{120x^{11}}{11} + \frac{24x^{10}}{5} + \frac{12x^7}{7} + 12x^{12} + 6x^6$$

$$= 67.972$$

7 Conclusion

A neighborhood NM-polynomial of a few medications related to the stomach was obtained and presented graphically in this research. The NM Polynomials of the ranitidine, omeprazole, and pantoprazole structures were first derived, followed by a few neighborhood degree-based topological indices. The primary benefit of NM-Polynomial is that several degree-based and neighborhood-based topological indices can be obtained from a single expression. One can investigate different chemical structures and derive an inference about them from their topological indices.

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