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On the Mostar Spectrum and Mostar Polynomials of Chemical Compounds

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Abstract The Mostar index is a bond-additive topological index that measures the degree of peripherality in graphs. Recently, the Mostar polynomial and Mostar matrix have been introduced as related concepts. In this paper, we compute the Mostar polynomial for specific classes of chemical compounds used in breast cancer treatment. From this, we derive explicit expressions for the Mostar index and hyper-Mostar index of these compounds. Furthermore, we calculate the Mostar spectra and Mostar energy for these compounds. Additionally, we perform a QSPR analysis to explore the relationship between Mostar energy and the physical properties of these chemical compounds.

1 Introduction

Breast cancer is the second-most common cancer in the world [3]. Recent research in this area has increased the survival rate, especially for women suffering from breast cancer. So more research about treatments and studies about the breast cancer treatment components will give more insight regarding the further developments on this area. In our study, we conducted a graph-theoretical analysis to give a better understanding of the compounds used for the treatment of breast cancer. Fourteen breast cancer medications were chosen for this analysis are given in Figure 1 [22]. Topological indices are numerical quantities associated with graphs that are invariant under graph isomorphism. Through the years, several variants of topological indices have been proposed and studied. Recently, Došlić *et al.* [24] proposed a new distance based graph invariant called the Mostar index to study the distance-balancedness of graphs. For a connected graph $G = (V, E)$, the Mostar index $Mo(G)$ is defined as

$$Mo(G) = \sum_{e=uv \in E} |n_u(e|G) - n_v(e|G)|$$

where $n_u(e|G)$ denote the number of vertices closer to the vertex u than v and vice versa. In analogous way, an edge variant called edge Mostar index was also proposed. For a graph $G = (V, E)$, the edge Mostar index [11] is defined as

$$Mo(G) = \sum_{e=uv \in E} |m_u(e|G) - m_v(e|G)|$$

where $m_u(e|G), m_v(e|G)$ are the edge counterparts of $n_u(e|G)$ and $n_v(e|G)$. Several new variants of Mostar indices have been proposed and studied, for more works on Mostar-related indices and topological indices of chemical structures, see [2, 4, 5, 6, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 25, 26, 27]. Associated with every relevant topological index, there exist associated polynomials. The most commonly studied polynomial associated with a topological

index is the Wiener polynomial (also called the Hosoya polynomial) [7, 18]. Analogous to the Wiener polynomial, a similar version of Mostar polynomial was proposed in [1]. Associated with this polynomial, a new index called hyper-Mostar index was also proposed. A similar version of polynomial and index can be proposed in the case of the edge version of Mostar index as well. Although, hyper-Mostar index has been proposed, it has not been studied properly. In this paper, we study the physical significance of hyper Mostar index for some compounds. We also propose the edge version of the Mostar polynomial and the corresponding hyper edge Mostar index. For a graph $G = (V, E)$, the edge Mostar polynomial is defined as

$$Mo_e(G : x) = \sum_{e=uv \in E} x^{|m_u(e|G) - m_v(e|G)|}$$

where $m_u(e|G)$ is the analogous edge version of $n_u(e|G)$. Then the hyper edge Mostar index $MMo_e(G)$ is defined as

$$MMo_e(G) = Mo'_e(G : 1) + \frac{1}{2}(Mo_e''(G : 1))$$

From the Mostar index, we can naturally define several associated square matrices to study the spectral variant of the Mostar index. An adjacency matrix with entries as the contribution of the edges of the Mostar index is called the Mostar Adjacency matrix, and the spectrum of the Mostar matrix is called the Mostar spectra. A similar version of matrices for the Szeged index has been proposed and studied in [8]. In order to study the mathematical properties of Mostar spectra, one has to identify whether or not the spectra and energy obtained from the Mostar matrix can be used as a measure for determining the physical properties of compounds. In this paper, we mean to understand the relevance of Mostar index, edge Mostar index, hyper Mostar index, hyper edge Mostar index, and Mostar energy in analyzing the physical properties of certain chemical compounds. Throughout this paper, we only consider simple, finite, undirected connected graphs. Therefore, we only consider the simple graphs associated with the chemical structures under consideration. For more details regarding the original structure of the compounds, see [22]. The following are some definitions that we will use throughout,

Definition 1. The **Mostar Polynomial** $Mo(G : x)$ of a graph G is defined as

$$Mo(G : x) = \sum_{e=uv \in E} x^{|n_u(e|G) - n_v(e|G)|}$$

Definition 2. The **Mostar index** is the derivative of Mostar Polynomial at x=1.

$$Mo(G) = Mo'(G : 1)$$

Definition 3. The **hyper-Mostar index** of a graph $G = (V, E)$ is

$$MMo(G) = Mo\prime(G : 1) + \frac{1}{2}(Mo\prime\prime(G : 1))$$

Definition 4. The **edge Mostar Polynomial** $Mo_e(G : x)$ of a graph G is defined as

$$Mo_e(G : x) = \sum_{e=uv \in E} x^{|m_u(e|G) - m_v(e|G)|}$$

Definition 5. The **edge-Mostar index** is the derivative of edge Mostar Polynomial at x=1. i.e,

$$Mo_e(G) = Mo'_e(G : 1).$$

Definition 6. The **hyper-edge Mostar index** of a graph $G = (V, E)$ is

$$MMo_e(G) = Mo_e\prime(G : 1) + \frac{1}{2}(Mo_e\prime\prime(G : 1))$$

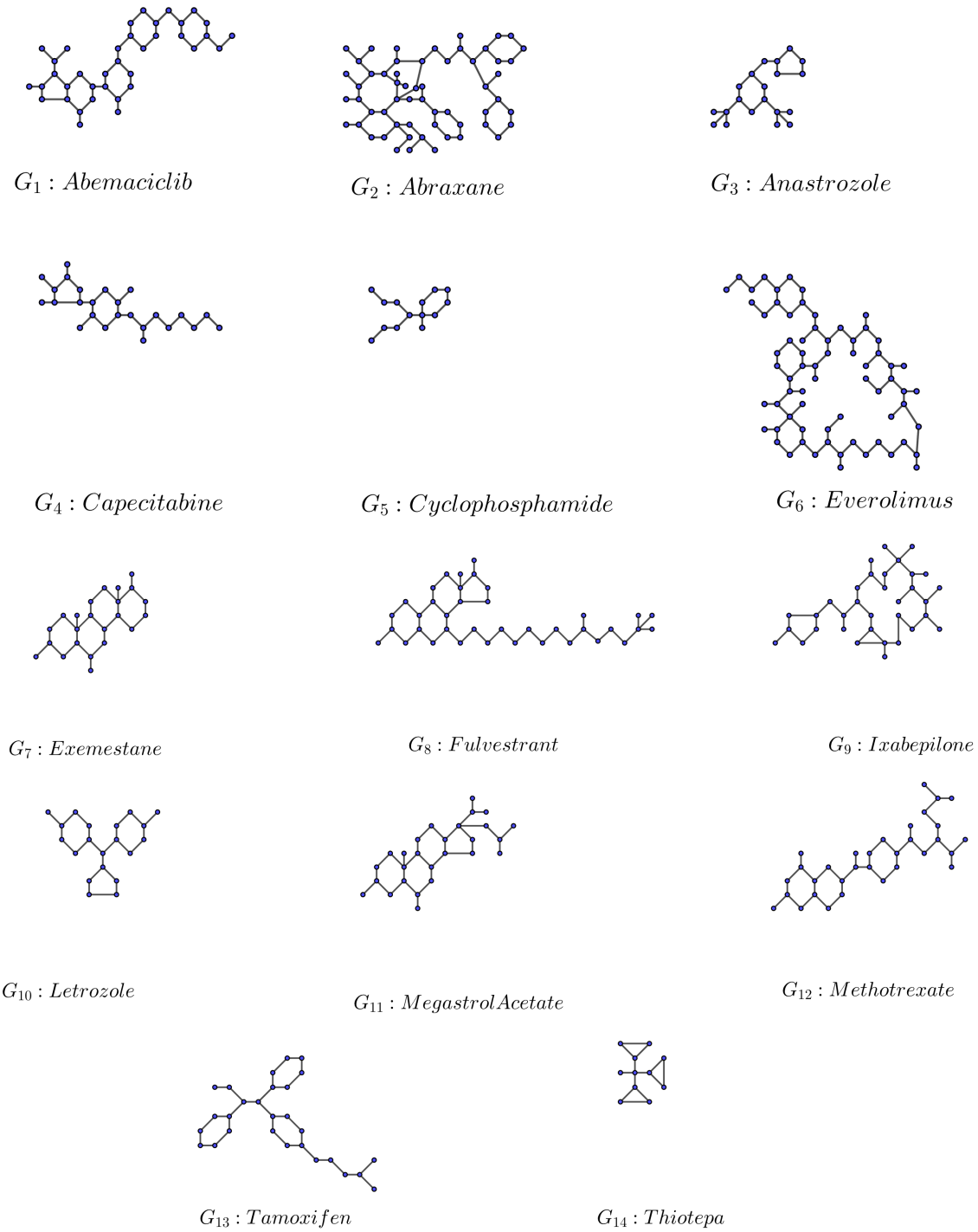

Figure 1: Graph theoretical structure of 14 compounds used for breast cancer treatment.

2 Main Results

In this section, we determine the Mostar polynomial of chemical compounds that are used for the treatment of breast cancer. All the compounds under discussion are plotted in Figure 1.

Theorem 2.1. *The Mostar polynomials of chemical compounds* $G_i, i = 1, 2, \ldots 5$ *are*

(1.) $Mo(G_1 : x) = 6x^{35} + x^{33} + x^{31} + 2x^{29} + 8x^{27} + 2x^{25} + x^{24} + x^{21} + x^{19} + 2x^{17} + 2x^{15} + 6x^{13} + x^9 + x^7 + x^5 + 5x$

(2.) $Mo(G_2 : x) = 15x^{57} + x^{55} + 20x^{53} + x^{51} + 2x^{49} + 3x^{47} + 2x^{43} + x^{41} + 2x^{39} + 6x^{35} + x^{29} + x^{25} + 3x^{23} + x^{21} + 2x^{13} + 3x^3$

(3.) $Mo(G_3 : x) = 6x^{18} + 4x^{15} + 2x^{12} + x^{10} + x^8 + 4x^6 + 2x^2 + 1$

(4.) $Mo(G_4 : x) = 7x^{23} + x^{21} + x^{19} + 2x^{17} + x^{16} + 3x^{15} + x^{13} + 2x^9 + x^7 + 7x$

(5.) $Mo(G_5 : x) = 3x^{12} + 2x^{10} + 8x^8 + 1$

Proof. In order to determine the Mostar polynomials of the compounds, we need to determine all the different possibilities for the contribution of the edges, and the number of edges corresponds to each contribution. The following table (Table 1) give a summary of the different values of the contributions and the number of edges corresponding to each contribution. Then, by the definition of the Mostar polynomials, the result follows.

Abemaciclib		Abraxane		Anastrozole		Capecitabine		Cyclophosphamide	
$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size
35	6	57	15	18	6	23	7	12	3
33	1	55	1	15	4	21	1	10	2
31	1	53	20	12	2	19	1	8	8
29	2	51	1	10	1	17	2	0	1
27	8	49	2	8	1	16	1		
25	2	47	3	6	4	15	3		
24	1	43	2	2	2	13	1		
21	1	41	1	0	1	9	2		
19	1	39	2			7	1		
17	2	35	6			1	7		
15	2	29	1						
13	6	25	1						
9	1	23	3						
7	1	21	1						
5	1	13	2						
1	5	3	3						

Table 1: The list of different values of $|n_u - n_v|$ and their corresponding size for different compounds.

□

Theorem 2.2. *The Mostar polynomials of chemical compounds* $G_i, i = 6, 7, \ldots 14$ *are*

(6.) $Mo(G_6 : x) = 18x^{66} + 4x^{64} + 5x^{62} + 3x^{60} + 2x^{54} + 4x^{50} + x^{44} + x^{42} + x^{38} + 2x^{23} + 3x^{22} + 5x^{21} + 2x^{20} + 2x^{19} + 7x^{18} + x^{17} + 4x^{14} + x^{11} + x^{10} + 3x^9 + x^6$

(7.) $Mo(G_7 : x) = 4x^{21} + 2x^{17} + 6x^{15} + 6x^9 + 2x^5 + 2x^3 + 4x$

(8.) $Mo(G_8 : x) = 7x^{36} + x^{32} + x^{31} + 5x^{30} + 2x^{28} + x^{26} + 2x^{25} + x^{24} + 4x^{22} + x^{20} + 4x^{18} + x^{16} + x^{14} + x^{12} + 4x^{10} + x^8 + x^6 + 2x^4 + x^2$

(9.) $Mo(G_9 : x) = 10x^{32} + x^{28} + 3x^{27} + x^{22} + x^{20} + x^{19} + x^{16} + 2x^{10} + 2x^8 + 3x^7 + 8x^6 + 2x^4 + x$

(10.) $Mo(G_{10} : x) = 2x^{18} + 4x^{15} + 12x^{12} + x^{10} + 2x^6 + 1$

(11.) $Mo(G_{11} : x) = 8x^{26} + 3x^{22} + 5x^{20} + x^{16} + 3x^{14} + x^9 + 2x^8 + 4x^6 + 2x^3 + 2$

(12.) $Mo(G_{12} : x) = 8x^{30} + 2x^{26} + 3x^{24} + 3x^{22} + 3x^{20} + 5x^{14} + x^{12} + 2x^8 + x^4 + 6x^2$

(13.) $Mo(G_{13} : x) = 3x^{26} + x^{24} + 13x^{22} + x^{20} + x^{18} + 3x^{16} + 7x^{10} + x^4$

(14.) $Mo(G_{14} : x) = x^9 + 6x^8 + 3x^5 + 3$

Proof. The result follows from Table 2,Table 3 and the definition of Mostar polynomial. □

Everolimus		Exemestane		Fulvestrant		Ixabepilone		Letrozole	
$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size
66	18	21	4	36	7	32	10	18	2
64	4	17	2	32	1	28	1	15	4
62	5	15	6	31	1	27	3	12	12
60	3	9	6	30	5	22	1	10	1
54	2	5	2	28	2	20	1	6	2
50	4	3	2	26	1	19	1	0	1
44	1	1	4	25	2	16	1		
42	1			24	1	10	2		
38	1			22	4	8	2		
23	2			20	1	7	3		
22	3			18	4	6	8		
21	5			16	1	4	2		
20	2			14	1	1	1		
19	2			12	1				
18	7			10	4				
17	1			8	1				
14	4			6	1				
11	1			4	2				
10	1			2	1				
9	3								
6	1								

Table 2: List of contribution of edges and their size

Megastrol Acetate		Methotrexate		Tamoxifen		Thiotepa	
$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size	$\|n_u - n_v\|$	size
26	8	30	8	26	3	9	1
22	3	26	2	24	1	8	6
20	5	24	3	22	13	5	3
16	1	22	3	20	1	0	3
14	3	20	3	18	1		
9	1	14	5	16	3		
8	2	12	1	10	7		
6	4	8	2	4	1		
3	2	4	1				
0	2	2	6				

Table 3: The values of $|n_u - n_v|$ and their corresponding size.

From the Mostar polynomials, we can directly compute the Mostar index of the corresponding components using definition 2.

Corollary 1. The Mostar index $Mo(G)$ of the chemical compounds $G_i, i = 1, 2 \ldots, 14$ are

$Mo(G_1) = 830$ $Mo(G_2) = 2854$ $Mo(G_3) = 238$ $Mo(G_4) = 341$ $Mo(G_5) = 120$
$Mo(G_6) = 2914$ $Mo(G_7) = 282$ $Mo(G_8) = 907$ $Mo(G_9) = 620$ $Mo(G_{10}) = 262$
$Mo(G_{11}) = 487$ $Mo(G_{12}) = 604 Mo(G_{13}) = 548$ $Mo(G_{14}) = 72$

Proof. Using the definition of the Mostar index and from Theorem 2.1 to Theorem 2.2. □

Abemaciclib		Abraxane		Anastrozole		Capecitabine		Cyclophosphamide	
$\lvert m_u - m_v\rvert$	size	$\lvert m_u - m_v\rvert$	size	$\lvert m_u - m_v\rvert$	size	$\lvert m_u - m_v\rvert$	size	$\lvert m_u - m_v\rvert$	size
40	6	63	15	20	6	25	7	13	3
38	1	61	1	16	4	23	1	11	2
36	1	59	2	14	2	21	1	9	2
33	1	58	18	10	1	19	1	8	6
31	7	57	1	8	1	18	1	1	1
29	1	54	2	7	4	17	2		
28	3	51	3	1	2	16	2		
24	1	47	2	0	1	15	1		
22	1	45	1			11	1		
21	1	44	2			9	2		
19	1	39	6			1	1		
17	2	31	1			0	6		
15	6	27	1						
10	1	26	2						
8	1	25	1						
6	1	23	1						
3	1	14	2						
1	4	1	3						
0	1								

Table 4: The edge contributions and the corresponding size.

Corollary 2. The Hyper-Mostar index of the chemical compounds $G_i, i = 1, 2, \ldots 14$ are

$MMo(G_1) = 11287$ $MMo(G_2) = 72227$ $MMo(G_3) = 1843$ $MMo(G_4) = 3371$

$MMo(G_5) = 632$ $MMo(G_6) = 79390$ $MMo(G_7) = 2266$ $MMo(G_8) = 12649$

$MMo(G_9) = 8064$ $MMo(G_{10}) = 1855$ $MMo(G_{11}) = 5281$ $MMo(G_{12}) = 7414$

$MMo(G_{13}) = 5826$ $MMo(G_{14}) = 306$

Proof. Using the definition of hyper Mostar index and from Theorem 2.1 to Theorem 2.2,. □

Using the same notion of Mostar polynomials in the case of edge versions, we can compute the edge Mostar polynomials and the corresponding indices.

Theorem 2.3. *The the edge- Mostar polynomial of* $G_i, i = 1, 2 \ldots 5$ *are*

(1.) $Mo_e(G_1 : x) = 6x^{40} + x^{38} + x^{36} + x^{33} + 7x^{31} + x^{29} + 3x^{28} + x^{24} + x^{22} + x^{21} + x^{19} + 2x^{17} + 6x^{15} + x^{10} + x^8 + x^6 + x^3 + 4x + 1$

(2.) $Mo_e(G_2 : x) = 15x^{63} + x^{61} + 2x^{59} + 18x^{58} + x^{57} + 2x^{54} + 3x^{51} + 2x^{47} + x^{45} + 2x^{44} + 6x^{39} + x^{31} + x^{27} + 2x^{26} + x^{25} + x^{23} + 2x^{14} + 3x$

(3.) $Mo_e(G_3 : x) = 6x^{20} + 4x^{16} + 2x^{14} + x^{10} + x^8 + 4x^7 + 2x + 1$

(4.) $Mo_e(G_4 : x) = 7x^{25} + x^{23} + x^{21} + x^{19} + x^{18} + 2x^{17} + 2x^{16} + x^{15} + x^{11} + 2x^9 + x + 6$

(5.) $Mo_e(G_5 : x) = 3x^{13} + 2x^{11} + 2x^9 + 6x^8 + x$

Proof. In order to determine the Mostar polynomials of the compounds, we need to determine all the different possibilities for the contribution of the edges, and the number of edges corresponds to each contribution. The following table (Table 4) gives a summary of the different values of the contributions and the number of edges corresponding to each contribution. □

Then the result follows from the definition of edge Mostar polynomial and from Table 5.

Theorem 2.4. *The the edge-Mostar polynomial of* $G_i, i = 6, \ldots 10$ *are*

(6.) $Mo_e(G_6 : x) = 16x^{70} + 2x^{69} + 4x^{68} + x^{66} + 4x^{65} + x^{64} + 2x^{63} + 2x^{57} + 4x^{53} + x^{46} + x^{44} + x^{40} + x^{26} + 4x^{25} + 5x^{24} + x^{23} + 3x^{22} + 2x^{20} + 5x^{19} + x^{18} + x^{16} + 3x^{14} + 2x^{10} + 4x^8$

(7.) $Mo_e(G_7 : x) = 5x^{25} + 2x^{20} + 6x^{18} + 6x^{11} + 2x^6 + 2x^4 + 3x$

(8.) $Mo_e(G_8 : x) = 7x^{40} + x^{35} + 2x^{34} + 4x^{33} + x^{32} + x^{31} + x^{30} + x^{28} + 2x^{27} + x^{24} + 4x^{23} + x^{22} + x^{20} + 4x^{18} + x^{16} + x^{14} + x^{12} + x^{10} + 4x^8 + x^6 + x^4$

(9.) $Mo_e(G_9 : x) = 10x^{35} + x^{31} + 3x^{29} + x^{23} + x^{22} + x^{21} + x^{17} + 2x^{10} + 12x^8 + 2x^6 + 2x$

(10.) $Mo_e(G_{10} : x) = 2x^{21} + 4x^{17} + 12x^{14} + x^{11} + 2x^7 + 1$

Everolimus		Exemestane		Fulvestrant		Ixabepilone		Letrozole	
$\|m_u - m_v\|$	size	$\|m_u - m_v\|$	size	$\|m_u - m_v\|$	size	$\|m_u - m_v\|$	size	$\|m_u - m_v\|$	size
70	16	25	5	40	7	35	10	21	2
69	2	20	2	35	1	31	1	17	4
68	4	18	6	34	2	29	3	14	12
66	1	11	6	33	4	23	1	11	1
65	4	6	2	32	1	22	1	7	2
64	1	4	2	31	1	21	1	0	1
63	2	1	3	30	1	17	1		
57	2			28	1	10	2		
53	4			27	2	8	12		
46	1			24	1	6	2		
44	1			23	4	1	2		
40	1			22	1				
26	1			20	1				
25	4			18	4				
24	5			16	1				
23	1			14	1				
22	3			12	1				
20	2			10	1				
19	5			8	4				
18	1			6	1				
16	1			4	1				
14	3								
10	2								
8	4								

Table 5: The edge contributions and the corresponding size.

Proof. The result follows from the definition of edge Mostar polynomial and Table 5. □

Theorem 2.5. *The the edge- Mostar polynomial of* $G_i, i = 11, 12, 13, 14$ *are*

(11.) $Mo_e(G_{11} : x) = 8x^{30}+2x^{26}+x^{25}+x^{24}+4x^{23}+x^{19}+3x^{16}+x^{12}+2x^9+x^8+3x^6+2x^5+2x$

(12.) $Mo_e(G_{12} : x) = 8x^{33} + 2x^{29} + x^{27} + 2x^{26} + x^{25} + 2x^{24} + 3x^{21} + x^{17} + x^{15} + 4x^{14} + x^{11} + x^7 + 6x^6 + x^3$

(13.) $Mo_e(G_{13} : x) = 3x^{29} + x^{27} + 13x^{24} + x^{23} + x^{21} + x^{19} + 2x^{17} + 6x^{12} + x^{11} + x^5$

(14.) $Mo_e(G_{14} : x) = x^{12} + 6x^{10} + 3x^6 + x^3 + 2$

Proof. The result follows from the definition edge Mostar polynomial and Table 6.

□

Corollary 3. The edge-Mostar index of the chemical compounds $G_i, i = 1, 2 \ldots, 14$ are

$Mo_e(G_1) = 918$ $Mo_e(G_2) = 3136$ $Mo_e(G_3) = 260$ $Mo_e(G_4) = 367$ $Mo_e(G_5) = 128$

$Mo_e(G_6) = 3100$ $Mo_e(G_7) = 362$ $Mo_e(G_8) = 1014$ $Mo_e(G_9) = 681$ $Mo_e(G_{10}) = 303$

$Mo_e(G_{11}) = 568$ $Mo_e(G_{12}) = 682$ $Mo_e(G_{13}) = 611$ $Mo_e(G_{14}) = 93$

Megastrol Acetate		Methotrexate		Tamoxifen		Thiotepa	
$\lvert m_u - m_v \rvert$	size	$\lvert m_u - m_v \rvert$	size	$\lvert m_u - m_v \rvert$	size	$\lvert m_u - m_v \rvert$	size
30	8	33	8	29	3	12	1
26	2	29	2	27	1	10	6
25	1	27	1	24	13	6	3
24	1	26	2	23	1	3	1
23	4	25	1	21	1	0	2
19	1	24	2	19	1		
16	3	21	3	17	2		
12	1	17	1	12	6		
9	2	15	1	11	1		
8	1	14	4	5	1		
6	3	11	1				
5	2	7	1				
1	2	6	6				
		3	1				

Table 6: The edge contributions and the corresponding size.

Proof. Using the definition of edge Mostar index and Theorem 2.3 to Theorem 2.5. □

Corollary 4. The Hyper-edge Mostar index of the chemical compounds $G_i, i = 1, 2 \ldots, 14$ are

$MMo_e(G_1) = 14135$ $MMo_e(G_2) = 87411$ $MMo_e(G_3) = 2219$ $MMo_e(G_4) = 3998$
$MMo_e(G_5) = 712$ $MMo_e(G_6) = 89230$ $MMo_e(G_7) = 3532$ $MMo_e(G_8) = 15555$
$MMo_e(G_9) = 9600$ $MMo_e(G_{10}) = 2456$ $MMo_e(G_{11}) = 7048$ $MMo_e(G_{12}) = 8975$
$MMo_e(G_{13}) = 7135$ $MMo_e(G_{14}) = 477$

Proof. The result follows from the definition hyper edge Mostar index and Theorem 2.3 to Theorem 2.5. □

Now we analyze the Mostar energy of the compounds under discussion. Let's recall the definitions of the Mostar adjacency matrix.

Definition 7. [1] The **Mostar adjacency matrix** is a symmetric,square $n \times n$ matrix A such that its element

$$A_{ij} = |n_i - n_j|$$

when there is an edge between vertex i and j and equal to 0 when there is no edge.

Definition 8. [1] The **characteristic polynomial of Mostar adjacency matrix** A is the polynomial defined as

$$\text{characteristic polynomial} = det(A - \lambda I)$$

where I denote the $n \times n$ identity matrix.

Definition 9. [1] The **Mostar energy** E_M of a graph is the sum of the absolute values of the eigenvalues of the Mostar adjacency matrix of the graph.i.e, if $\lambda_i, i = 1, 2, \ldots, n$ are the eigenvalues of A, then

$$E_M(G) = \sum |\lambda_i|$$

Example 2.6. For example, consider a path P_4. The corresponding Mostar adjacency matrix is

$$A = \begin{bmatrix} 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{bmatrix}$$

Then its Mostar polynomial is $det(A - \lambda I) = \lambda^4 - 8\lambda^2 + 16$ and the corresponding eigenvalues are $-2, 2$ each, with multiplicity 2. Therefore, the energy $E_M = 8$.

Similarly, we can directly compute the Mostar energy of the 14 compounds we have discussed.

Theorem 2.7. *The Mostar energy of the chemical compounds $G_i, i = 1, 2, \ldots, 14$ are*

$$E_M(G_1) = 1042.407554 \quad E_M(G_2) = 3496.759074 \quad E_M(G_3) = 264.8295104$$
$$E_M(G_4) = 508.979545 \quad E_M(G_5) = 157.4301245 \quad E_M(G_6) = 3430.339585$$
$$E_M(G_7) = 372.2906874 \quad E_M(G_8) = 1201.047814 \quad E_M(G_9) = 954.6340627$$
$$E_M(G_{10}) = 326.3591764 \quad E_M(G_{11}) = 613.4915984 \quad E_M(G_{12}) = 722.8576078$$
$$E_M(G_{13}) = 680.8572438 \quad E_M(G_{14}) = 89.42028443$$

Proof. From direct computation, we can obtain the characteristic polynomials of the compounds. From these polynomials we can directly compute the Mostar spectrum and Mostar energy of the corresponding components. □

Using the characteristic polynomials of from Mostar matrix, we have the following corollary.

Corollary 5. Zero is an eigenvalue for all the Mostar adjacency matrix for all the graphs $G_i, i = 1, 2, \ldots, 14$.

3 Application of Mostar index and Mostar Energy

This section explores the application of distance-based topological indices in analyzing medications used for breast cancer treatment. We investigate the correlation between these topological indices and the physical properties of the constituent chemical compounds. Fourteen breast cancer medications were chosen for this analysis: Abemaciclib, Abraxane, Anastrozole, Capecitabine, Cyclophosphamide, Everolimus, Exemestane, Fulvestrant, Ixabepilone, Letrozole, Megestrol Acetate, Methotrexate, Tamoxifen, and Thiotepa. Their molecular structures, depicted in Figure 1, are represented as graphs, where atoms are vertices and bonds between them are edges.

Sl. No.	Name	Mo	MMo	BP	MP(C)	EV	FP(C)	MR	MV(cm3)	P
1	Abemaciclib	830	11287	689.3		101	307.7	104.4	382.3	55.7
2	Abraxane	2854	72227	957.1		146	532.6	219.3	610.6	86.9
3	Anastrozole	238	1843	469.7	81.5	73.2	237.9	90	270.3	35.7
4	Capecitabine	341	3371	517	115.5			82.3	240.5	32.6
5	Cyclophosphamide	120	632	336.1	51	57.9	157.1	58.1	195.7	23
6	Everolimus	2914	79390	998.7	998.7	165.1	557.8	257.7	811.2	102.2
7	Exemestane	282	2266	453.7	155.13	71.3	169	85.8	260.2	34
8	Fulvestrant	907	12649	674.8	104	104.1	361.9	154	505.1	61.1
9	Ixabepilone	620	8064	697.8		107.3	375.8	140.1	451.6	55.5
10	Letrozole	262	1855	563.5	181	84.7	294.6	87.1	234.5	34.5
11	Megestrol Acetate	487	5281	507.1	214	77.7	77.7	106.4	333.4	42.2
12	Methotrexate	604	7414		192			119	295.7	47.2
13	Tamoxifen	548	5826	482.3	96	74.7	140	118.9	118.9	47.1
14	Thiotapa	72	306	270.2	51.5	50.8	117.2	49.1	125.8	19.5

Table 7: The table contains the value of Mostar index, Hyper Mostar index, Boiling point (BP), Melting point (MP), Enthalpy of Vaporization (EV), Flash Point (FP), Molar Refractivity(MR), Molar Volume(MV), Polarizability(P) of breast cancer treatment compounds.

Table 7 and graphs (Figure 1) give the values of the Mostar index and hyper-Mostar index of the 14 breast cancer treatment compounds. Table 8 gives the values of the edge Mostar index

Sl. No.	Name	Mo_e	MMo_e	BP	MP(C)	EV	FP(C)	MR	MV(cm3)	P
1	Abemaciclib	918	14135	689.3		101	307.7	104.4	382.3	55.7
2	Abraxane	3136	87411	957.1		146	532.6	219.3	610.6	86.9
3	Anastrozole	260	2219	469.7	81.5	73.2	237.9	90	270.3	35.7
4	Capecitabine	367	3998	517	115.5			82.3	240.5	32.6
5	Cyclophosphamide	128	712	336.1	51	57.9	157.1	58.1	195.7	23
6	Everolimus	3100	89230	998.7	998.7	165.1	557.8	257.7	811.2	102.2
7	Exemestane	362	3532	453.7	155.13	71.3	169	85.8	260.2	34
8	Fulvestrant	1014	15555	674.8	104	104.1	361.9	154	505.1	61.1
9	Ixabepilone	681	9600	697.8		107.3	375.8	140.1	451.6	55.5
10	Letrozole	303	2456	563.5	181	84.7	294.6	87.1	234.5	34.5
11	Megestrol Acetate	568	7048	507.1	214	77.7	77.7	106.4	333.4	42.2
12	Methotrexate	682	8975		192			119	295.7	47.2
13	Tamoxifen	548	5826	482.3	96	74.7	140	118.9	118.9	47.1
14	Thiotapa	93	447	270.2	51.5	50.8	117.2	49.1	125.8	19.5

Table 8: The table contains the value of edge Mostar index, Hyper edge Mostar index, Boiling point (BP), Melting point (MP), Enthalpy of Vaporization (EV), Flash Point (FP), Molar Refractivity(MR), Molar Volume(MV), Polarizability(P) of breast cancer treatment compounds.

Sl. No.	Name	E_M	BP	MP	EV	FP	MR	MV(cm3)	P
1	Abemaciclib	1042.407554	689.3		101	307.7	104.4	382.3	55.7
2	Abraxane	3496.759074	957.1		146	532.6	219.3	610.6	86.9
3	Anastrozole	264.8295104	469.7	81.5	73.2	237.9	90	270.3	35.7
4	Capecitabine	508.979545	517	115.5			82.3	240.5	32.6
5	Cyclophosphamide	157.4301245	336.1	51	57.9	157.1	58.1	195.7	23
6	Everolimus	3430.339585	998.7	998.7	165.1	557.8	257.7	811.2	102.2
7	Exemestane	372.2906874	453.7	155.13	71.3	169	85.8	260.2	34
8	Fulvestrant	1201.047814	674.8	104	104.1	361.9	154	505.1	61.1
9	Ixabepilone	954.6340627	697.8		107.3	375.8	140.1	451.6	55.5
10	Letrozole	326.3591764	563.5	181	84.7	294.6	87.1	234.5	34.5
11	Megestrol Acetate	613.4915984	507.1	214	77.7	77.7	106.4	333.4	42.2
12	Methotrexate	722.8576078		192			119	295.7	47.2
13	Tamoxifen	680.8572438	482.3	96	74.7	140	118.9	118.9	47.1
14	Thiotapa	89.42028443	270.2	51.5	50.8	117.2	49.1	125.8	19.5

Table 9: The table contains the value of Mostar Energy, Boiling point (BP), Melting point (MP), Enthalpy of Vaporization (EV), Flash Point (FP), Molar Refractivity(MR), Molar Volume(MV), Polarizability(P) of breast cancer treatment compounds.

and hyper edge Mostar index of these compounds, and Table 9 gives the values of the Mostar energy of the compounds. We obtained the correlation between the five topological descriptors of these compounds and the boiling point (BP), melting point (MP), enthalpy of vaporization (EV), flash point (FP), molar refractivity (MR), molar volume (MV), and polarizability (P) of the compounds. Table 8 gives a summary of the correlation between these parameters. We obtain that the Mostar index has a high correlation with Boiling point(0.9145),Melting point (0.9557), Enthalpy of vaporization (0.9429), Molar refractivity (0.9494), and Polarizability (0.9500). The hyper Mostar index has a high linear correlation with Melting point (0.9757), Enthalpy of vaporization (0.9143), Molar refractivity (0.9215) and Polarizability (0.9130). The edge Mostar index has a high linear relationship with Boiling point (0,9145), Melting point (9539), Enthalpy of vaporization (0.9410), Molar refractivity (0.9483) and Polarizabilty (0.9491). The hyper-edge Mostar index has a high linear correlation with Melting point (0.9754), Enthalpy of vaporization (0.9124), Molar refractivity (0.9189) and Polarizability (0.9114). Mostar energy has a high linear correlation with Boiling point (0.9267), Melting point (0.9456), Enthalpy of vaporiza-

Property/Index	Mo	MMo	Mo_e	MMo_e	E_M
BP	0.9145	0.8727	0.9145	0.8748	**0.9267**
MP	0.9557	**0.9757**	0.9539	0.9754	0.9456
EV	0.9429	0.9143	0.9410	0.9124	**0.9510**
FP	0.8593	0.8389	0.8564	0.8385	**0.8715**
MR	0.9494	0.9215	0.9483	0.9189	**0.9540**
MV	0.8882	0.8661	0.8857	0.8613	**0.8963**
P	0.9500	0.9130	0.9491	0.9114	**0.9548**

Table 10: The table contains the value of correlation between Mostar index (Mo), hyper Mostar index (MMo), edge Mostar index (Mo_e), hyper edge Mostar index (MMo_e), Mostar Energy (E_M) and Boiling point (BP), Melting point (MP), Enthalpy of Vaporization (EV), Flash Point (FP), Molar Refractivity(MR), Molar Volume(MV), Polarizability(P) of breast cancer treatment compounds.

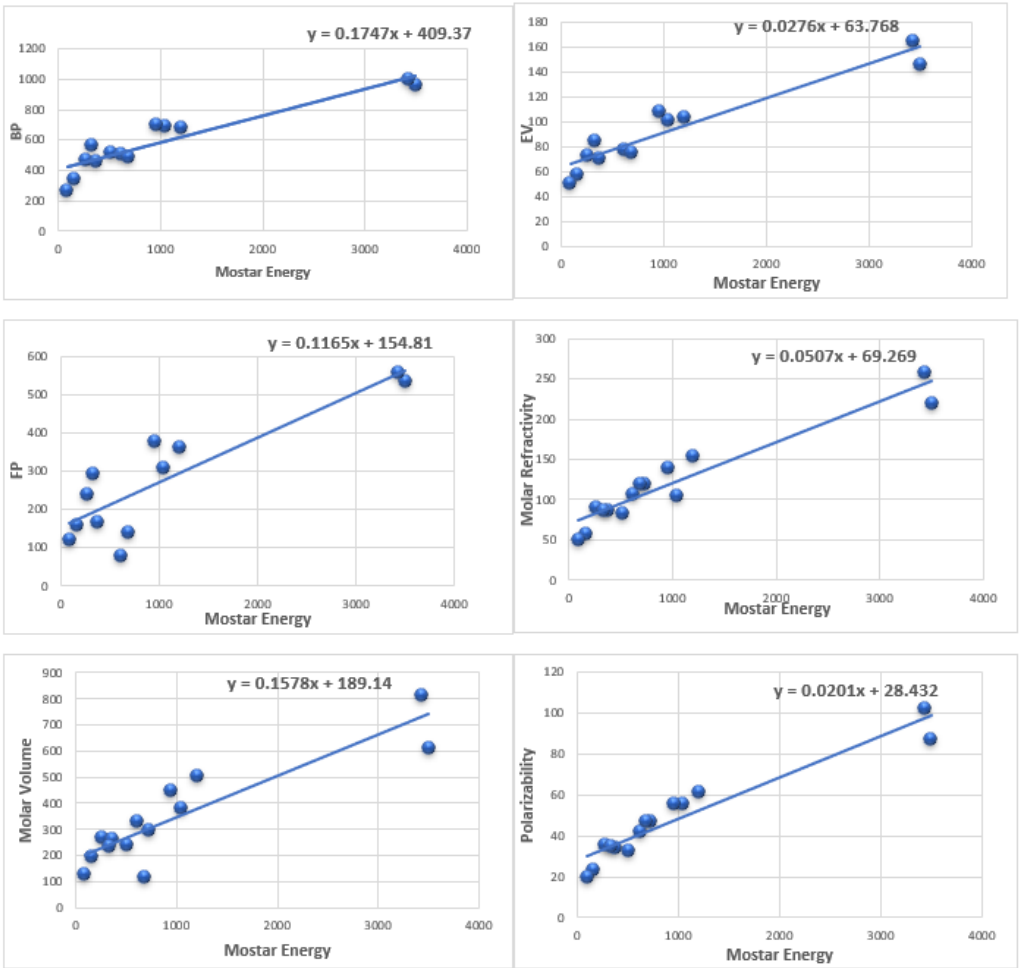

Figure 2: Scatter plots of Mostar energy versus Boiling point (BP), Melting point (MP), Enthalpy of Vaporization (EV), Flash Point (FP), Molar Refractivity(MR), Molar Volume(MV), Polarizability(P) of breast cancer treatment compounds.

tion (0.9510), Molar refractivity (0.9540), Molar volume (0.8963), and Polarizabilty (0.9548). Among the five topological descriptors, Mostar energy has the highest relationship with six physical properties compared to the other descriptors. The hyper Mostar index has the highest

correlation with Melting point. The relationship indicates that the Mostar energy is a better predictor for multiple properties of these chemical compounds compared to the other descriptors. Thereby establishing its significance among other structural descriptors. Although other structural descriptors have been used to study physical properties in [4, 5, 22], no single structural descriptor has been identified as a superior predictor for multiple physical properties. However, we have found that Mostar energy can serve as a better predictor for multiple physical properties.

We have used linear regression model

$$PP = \beta(TI) + \alpha$$

where PP is the physical property, α is the constant, β is the regression coefficient and TI is the topological index. The constant α and the regression coefficient β have been computed using SPSS. We have determined the linear regression equations of the physical properties of the compounds, with the topological descriptor having the highest correlation with the property. The following are the linear regression equations:

$$\begin{aligned} BP &= 0.1747(E_M) + 409.37 \\ MP &= 0.0114(MMo) + 77.954 \\ EV &= 0.0276(E_M) + 63.768 \\ FP &= 0.1165(E_M) + 154.81 \\ MR &= 0.0507(E_M) + 69.269 \\ MV &= 0.1578(E_M) + 189.14 \\ P &= 0.0201(E_M) + 28.432 \end{aligned}$$

4 Conclusion

In this paper, we investigate the application of several graph-based descriptors to 14 chemical compounds relevant to breast cancer research. We computed the Mostar polynomial, edge Mostar polynomial, Mostar index, edge Mostar index, and Mostar energy for each compound. Furthermore, we explored the physical significance of these descriptors, aiming to establish their potential for understanding the compounds' properties. Our analysis revealed significant correlations between various distance-based topological indices and the physical properties of 14 breast cancer treatment compounds. Notably, Mostar energy exhibited the strongest linear relationship with these properties compared to other descriptors. This unique characteristic, where a single descriptor correlates with multiple properties, highlights the importance of Mostar energy in QSPR analysis. These findings strongly suggest that Mostar energy is a powerful structural descriptor. This knowledge can be instrumental for medicinal chemists in designing new drugs by leveraging insights from existing, highly correlated breast cancer treatments.

Furthermore, this study paves the way for a broader application. By establishing relationships between physical properties, drugs, and topological indices, we can estimate the properties of newly discovered drugs for various diseases. Given the remarkable significance of Mostar energy as a structural descriptor, this work opens doors for future research into its mathematical properties. This exploration could encompass various classes of graphs and structures, potentially leading to a deeper understanding of its applicability.

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