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Stability and Maximum Independent Bond Set Polynomials of Painkiller Molecules Using Maximum Matching

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Abstract. Chemical graph theory establishes a connection between the properties of molecules and their corresponding molecular graphs. A topological index is a graph invariant that characterizes the graph's structure and remains unaffected by graph automorphisms. In chemical graph theory, degree-based topological indices are particularly significant, offering crucial insights into the structural features of molecules. In this work, we introduce the maximum independent bond set polynomial $MIBSP(H; x, y)$, a powerful tool for deriving various degree-based topological indices. We specifically apply $MIBSP(H; x, y)$, to the chemical graphs of several painkiller molecules, including Aspirin, Paracetamol, Caffeine, Ibuprofen, Phenacetin, and Salicylic acid. The degree-based topological indices derived from these polynomials provide a deeper understanding of the molecular structures and their potential applications in pharmaceutical research.

2020 Mathematics Subject Classifications: 05C05, 05C07, 05C10, 94C15
Key Words and Phrases: Kekule Structure, Maximum matching, Graph Polynomials, Topological indices, Painkiller

1. Introduction

Pain is an undesirable sensation that can run from gentle, limited uneasiness to misery. Pain is an inherent aspect of daily life for humans and remains one of the oldest challenges in the field of medicine. The most widely used approach for managing pain is medication, and in recent times, there has been a noticeable rise in the use of analgesics. This increase is largely driven by factors such as growing self-medication habits and greater availability of over-the-counter (OTC) drugs [1–4]. Analgesics are currently among the most widely used drugs globally, with millions of individuals estimated to take over-the-counter (OTC) painkillers on a daily basis [5, 6]. The use of analgesics may have effects that extend beyond simply alleviating pain, as changes in psychological and social factors such as diminished responses to emotionally charged images and decreased reports of social pain have been observed with analgesic use [7, 8].

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Pain is a complex, subjective experience that encompasses physical, psychological, and social dimensions. Pain can originate from various causes, such as injury, illness, inflammation, and nerve damage [9]. It can significantly impact an individual's overall quality of life, hindering their ability to carry out daily tasks, meet work responsibilities, and engage in social activities [10, 11]. The process of sensing pain involves the activation of sensory neurons, the conduction of electrical and chemical signals through neural pathways, and the interpretation of these signals by regions of the brain responsible for higher functions [12, 13]. The creation and regulation of pain sensation are influenced by a variety of mechanisms [14]. As seen in studies like that of Hargreave et al. [15], this study also supports the notion of a gender disparity in analgesic consumption. Among the 54.0% of students who reported using analgesics, 36.0% were female, while 18.0% were male.

Chemical graph theory plays a significant role in the study of chemical structures, representing them as molecular graphs where vertices correspond to atoms and edges represent bonds. These molecular graphs are used to derive molecular descriptors or topological indices, which are numerical values that predict the physical, chemical, and biological properties of molecules [16, 17]. The concept of topological indices was first applied to study the physical properties of chemical structures in 1947 [18]. These indices play a crucial role in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies, which are essential for predicting the bioactivity and physicochemical properties of novel drug molecules.

Molecular descriptors are based on factors such as the vertex degree of the graph, the distance between vertices, the eigenvalues of the graph, and other related properties. Using topological polynomials, rather than calculating molecular descriptors individually, simplifies the process of providing details regarding the molecular graph. M-polynomials are formulas derived from molecular descriptors that depend on the vertex degrees of a graph G, as defined in [19]. Building on this definition, NM-polynomials are also introduced. These polynomials are influenced by the sum of the degrees of adjacent vertices [20, 21]. Cycle-related graphs represent the molecular structures of various chemical compounds, such as cycloalkanes, and are also used as graph representations for many types of networks [22]. Total-eccentricity polynomials were examined in [23]. The calculation of the Mostar index for cycle-related chemical structures was performed in [24]. Topological numbers in a uniform intuitionistic fuzzy environment and their application in neural networks were explored in [25]. The determination of Leap-Zagreb indices for cycle-related special graphs was conducted in [26], and the M-polynomials of cycle-related graphs were explored in [27]. The edge-Mostar index and Mostar index of cycle-related graphs were computed in [28], while the reciprocal-leap indices of wheel graphs were studied in [29]. Topological numbers of fuzzy soft graphs and their applications in globalizing the world through mutual trade are discussed in [30]. The precise values for the Randic, Zagreb, Harmonic, Augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices of Benzenoid networks were studied in [31].

A notable concept in chemical graph theory is the Kekulé structure, introduced by F.A. Kekulé to describe the resonance forms of aromatic compounds [32]. These structures illustrate alternating single and double bonds in conjugated systems, such as the

benzene ring. Kekulé structures are fundamentally linked to the stability and resonance energy of aromatic compounds because they depict the delocalization of π-electrons across the molecule [33, 34]. For example, benzene possesses multiple Kekulé structures, a feature that significantly contributes to its exceptional stability and aromatic character. The proposed MIBSP advances chemical graph theory by unifying two previously disjoint approaches: (1) degree-based indices (e.g., Zagreb, Randic) that ignore bond arrangements, and (2) matching enumerations (e.g., Hosoya index) that disregard vertex degrees. Unlike M-polynomials which capture degree correlations but not matchings or Kekulé structures restricted to alternant hydrocarbons, MIBSP's polynomial formulation simultaneously encodes both features through its edge-weighted matching sum .

2. Key Concepts and Background Literature

Throughout this article, suppose $H(V(H), E(H))$ is an undirected graph of a chemical structure, $V(H)$ represent the set of vertices and $E(H)$ represent the set of edges. Number of vertices incident with u in a graph H is called degree of u denoted by d_u or $d_H(u)$. The minimum and maximum degree in H denoted by δ and Δ, respectively. A subset X of the edge set of a graph H is called independent if no two edges of X are adjacent in H. A matching in a graph H is a set of independent edges X. A maximal matching in a graph H is a matching that cannot be enlarged by adding another edge because the edges are incident to some independent edges. A matching X in a graph H is a maximum matching if H contains no matching X' with $|X'| > |X|$. The cardinality of the maximum matching in H is referred to as the matching number of H denoted by $\beta(H)$ [35].

In graph theory, a matching in a graph H consists of independent edges with no shared vertices. This concept mirrors the Kekulé structure of aromatic compounds, where alternating single and double bonds represent independent bonding interactions. Each independent edge in the matching corresponds to one alternating bond in the Kekulé structure. By applying perfect matchings to Kekulé structures, we can quantify the delocalization and stability of bonding interactions in aromatic compounds, offering insights into their resonance behavior and structural stability.

Definition 1. *[19] Consider H as a simple, connected and undirected graph. The M-polynomial for H is defined as follows:*

$$M(H; x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{i,j} x^i y^j,$$

where $m_{i,j}$ denotes the number of edges $e = uv \in E(H)$ such that $\{d_H(u), d_H(v)\} = \{i, j\}$.

We define the maximum independent bond set polynomials as:

Definition 2. *Let H be a simple undirected graph of order p and size q. Then the maximum independent bond set polynomial of H is defined as:*

$$MIBSP(H;x,y)=\sum_{r=1}^{\alpha}\sum_{\substack{\forall uv\in X_r\\ \delta\le i\le j\le\Delta}} m_{i,j}x^iy^j,$$

where α is the number of maximum matchings in H, X_r, $r=1,2,...,\alpha$ are the sets of maximum matchings in H, and $m_{i,j}$ denotes the number of edges $e=uv\in E(H)$ such that $\{d_H(u),d_H(v)\}=\{i,j\}$.

Our definition can be rephrased in another way

$$MIBSP(H;x,y)=\sum_{r=1}^{\alpha}M(X_r(H);x,y),$$

where α is the number of maximum matchings in H, X_r, $r=1,2,...,\alpha$ are the sets of maximum matchings in H, and $M(X_r(H);x,y)$ is the M-polynomial of a maximum matchings X_r for $r=1,2,...,\alpha$.

The Maximum Independent Bond Set Polynomial (MIBSP) is the first method to combine maximum matchings with degree-based indices, introducing novel descriptors (e.g. $\mathcal{M}M_1(H)$, $\mathcal{M}M_2(H)$) for chemical graph analysis. It unifies bonding patterns and structural features, enhancing drug stability prediction (e.g., Caffeine's perfect matching) and materials science applications like graphene studies. MIBSP outperforms traditional indices by quantifying bond sets that Kekulé structures and topological indices miss, offering new QSAR/QSPR capabilities.

The first Zagreb index, denoted by M_1, and the second Zagreb index, denoted by M_2, are introduced in [36], and are defined as follows:

$$M_1(H)=\sum_{uv\in E(H)}(d_u+d_v),$$
$$M_2(H)=\sum_{uv\in E(H)}(d_ud_v).$$

The general Randic index was introduced in [37],

$$R_\gamma(H)=\sum_{uv\in E(H)}(d_ud_v)^\gamma.$$

Harmonic index defined in [38], and the inverse sum index established in [39],

$$\mathrm{H}(H)=\sum_{uv\in E(H)}\tfrac{2}{d_u+d_v},$$

$$I(H)=\sum_{uv\in E(H)}\tfrac{d_ud_v}{d_u+d_v}.$$

Symmetric division degree index $SSD(H)$, introduced in [40] formulated as:

$$SSD(H)=\sum_{uv\in E(H)}(\tfrac{Min(d_u,d_v)}{Max(d_u,d_v)}+\tfrac{Max(d_u,d_v)}{Min(d_u,d_v)}).$$

The following Table 1 enlisted some standard topological indices based on degrees of maximum independent bond set and their derivation from the maximum independent bond set polynomials, where $D_x = x\frac{\partial f(x,y)}{\partial x}$, $D_y = y\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(x,y)}{t}dt$, $S_y = \int_0^y \frac{f(x,y)}{t}dt$, $Jf(x,y) = f(x,x)$.

Table 1: Matching degree-based topological indices: their formulas and derivations from $MIBSP(H;x,y)$.

Matching degree-based topological indices	Formula	Derivation from $MIBSP(H;x,y)$
$\mathcal{M}M_1(H)$	$\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(d_u+d_v) = \sum_{r=1}^{\alpha} M_1(X_r)$	$(D_x+D_y)MIBSP(H)\|_{x=y=1}$
$\mathcal{M}M_2(H)$	$\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(d_u d_v) = \sum_{r=1}^{\alpha} M_2(X_r)$	$(D_xD_y)MIBSP(H)\|_{x=y=1}$
$\mathcal{M}R_\gamma(H)$	$\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(d_u d_v)^\gamma = \sum_{r=1}^{\alpha} R_\gamma(X_r)$	$(D_x^\gamma+D_y^\gamma)MIBSP(H)\|_{x=y=1}$
$\mathcal{M}\mathrm{H}(H)$	$\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}\frac{2}{d_u+d_v} = \sum_{r=1}^{\alpha} H(X_r)$	$(2S_xJ)MIBSP(H)\|_{x=y=1}$
$\mathcal{M}\mathrm{I}(H)$	$\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}\frac{d_u d_v}{d_u+d_v} = \sum_{r=1}^{\alpha} I(X_r)$	$(S_xJD_xD_y)MIBSP(H)\|_{x=y=1}$
$\mathcal{M}\mathrm{SSD}(H)$	$\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(\frac{Min(d_u,d_v)}{Max(d_u,d_v)}+\frac{Max(d_u,d_v)}{Min(d_u,d_v)}) = \sum_{r=1}^{\alpha} SSD(X_r)$	$(S_yD_x+S_xD_y)MIBSP(H)\|_{x=y=1}$

3. Main Results

This section divided in to two subsections.

3.1. Derivations of Matching Degree-Based Topological Indices

In this subsection, we give proofs of closed formulas mentioned in Table 1. Given $uv \in E(H)$, with $d_u \le d_v$, the operations D_x, D_y, D_x^γ, D_y^γ, S_x, S_y, I and J defined on $MIBSP(H;x,y)$, are given by:

- $D_x(MIBSP(H;x,y)) = x\frac{\partial}{\partial(x)}(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} x^{d_u}y^{d_v})$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_u x^{d_u}y^{d_v}.$$

- $D_x^2(MIBSP(H;x,y)) = x\frac{\partial}{\partial(x)}(x\frac{\partial}{\partial(x)}(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} x^{d_u}y^{d_v}))$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_u^2 x^{d_u} y^{d_v}.$$

- $D_xD_y(MIBSP(H;x,y)) = x\frac{\partial}{\partial(x)}(y\frac{\partial}{\partial(y)}(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} x^{d_u}y^{d_v}))$

$$=x\frac{\partial}{\partial(x)}(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_v x^{d_u}y^{d_v})$$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_u d_v x^{d_u}y^{d_v}.$$

- $S_x(MIBSP(H;x,y)) = S_x(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} x^{d_u}y^{d_v})$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} \frac{1}{d_u} x^{d_u}y^{d_v}.$$

- $D_x^{\gamma}(MIBSP(H;x,y)) = D_x^{\gamma}(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} x^{d_u}y^{d_v})$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_u^{\gamma} x^{d_u}y^{d_v}.$$

- $J(MIBSP(H;x,y)) = MIBSP(H;x,x)$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} x^{d_u+d_v}.$$

Similarly,

- $D_y(MIBSP(H;x,y)) = \sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_v x^{d_u}y^{d_v}.$
- $D_y^2(MIBSP(H;x,y)) = \sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_v^2 x^{d_u}y^{d_v}.$
- $S_y(MIBSP(H;x,y)) = \sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} \frac{1}{d_v} x^{d_u}y^{d_v}.$
- $D_y^{\gamma}(MIBSP(H;x,y)) = \sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r} d_v^{\gamma} x^{d_u}y^{d_v}.$

The matching degree-based topological indices are given in the following theorem.

Theorem 1. *Let $MIBSP(H;x,y)$ denote the maximum independent bond set polynomial of a graph H. Then, the matching degree-based topological indices are given by:*

(i) The matching first Zagreb index is given by:

$$\mathcal{M}M_1(H) = (D_x + D_y)MIBSP(H; x, y)|_{x=y=1}.$$

(ii) The matching second Zagreb index is given by:

$$\mathcal{M}M_2(H) = (D_xD_y)MIBSP(H; x, y)|_{x=y=1}$$

(iii) The matching general Randic index is given by:

$$\mathcal{M}R_\gamma(H) = (D_x^\gamma D_y^\gamma)MIBSP(H; x, y)|_{x=y=1}$$

(iv) The matching Harmonic index is given by:

$$\mathcal{M}\mathrm{H}(H) = (2S_xJ)MIBSP(H; x, y)|_{x=y=1}$$

(v) The matching Inverse index is given by:

$$\mathcal{M}\mathrm{I}(H) = (S_xJ)(D_xD_y)MIBSP(H; x, y)|_{x=y=1}$$

(vi) The matching Symmetric Division index is given by:

$$\mathcal{M}\mathrm{SSD}(H) = (S_yD_x + S_xD_y)MIBSP(H; x, y)|_{x=y=1}$$

Proof. Let $uv \in E(H)$ with $d_u \leq d_v$, then by definition 2, we get

(i) $$\begin{aligned}(D_x + D_y)(MIBSP(H; x, y)) &= (D_x + D_y)(\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v}) \\ &= D_x(\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v}) + D_y(\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v}) \\ &= \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} d_u x^{d_u} y^{d_v} + \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} d_v x^{d_u} y^{d_v} \\ &= \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u + d_v) x^{d_u} y^{d_v}.\end{aligned}$$

Therefore, $\mathcal{M}M_1(H) = (D_x + D_y)MIBSP(H; x, y)|_{x=y=1} = \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u + d_v)$.

(ii) $$\begin{aligned}(D_xD_y)(MIBSP(H; x, y)) &= (D_xD_y)(\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v}) \\ &= D_x(D_y \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v})\end{aligned}$$

$$=D_x \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} d_v x^{d_u} y^{d_v}$$

$$=\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u d_v) x^{d_u} y^{d_v}.$$

Therefore, $\mathcal{M}M_2(H) = (D_x D_y) MIBSP(H; x, y)|_{x=y=1} = \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u d_v)$.

(iii) $(D_x^{\gamma} D_y^{\gamma})(MIBSP(H; x, y)) = (D_x^{\gamma} D_y^{\gamma})(\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v})$

$$=D_x^{\gamma}(D_y^{\gamma} \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v})$$

$$=D_x^{\gamma} \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} d_v^{\gamma} x^{d_u} y^{d_v}$$

$$=\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u^{\gamma} d_v^{\gamma}) x^{d_u} y^{d_v}.$$

Therefore, $\mathcal{M}R_{\gamma}(H) = (D_x^{\gamma} D_y^{\gamma}) MIBSP(H; x, y)|_{x=y=1} = \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u d_v)^{\gamma}$.

(iv) $(2S_x J) MIBSP(H; x, y) = (2S_x) J \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v})$

$$=2S_x(\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u + d_v})$$

$$=2 \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} \frac{1}{d_u + d_v} x^{d_u + d_v}$$

$$=\sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} \frac{2}{d_u + d_v} x^{d_u + d_v}$$

Therefore, $\mathcal{M}\mathrm{H}(H) = (2S_x J) MIBSP(H; x, y)|_{x=y=1} = \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} \frac{2}{d_u + d_v}$.

(v) $(S_x J)(D_x D_y) MIBSP(H; x, y) = (S_x J)(D_x(D_y \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} x^{d_u} y^{d_v}))$

$$=(S_x J) D_x \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} d_v x^{d_u} y^{d_v}$$

$$=(S_x(J \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u d_v) x^{d_u} y^{d_v}))$$

$$=S_x \sum_{r=1}^{\alpha} \sum_{\forall uv \in X_r} (d_u d_v) x^{d_u + d_v}$$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(\tfrac{d_u d_v}{d_u+d_v})x^{d_u+d_v}.$$

Therefore, $\mathcal{M}\mathrm{I}(H)=(S_xJ)(D_xD_y)MIBSP(H;x,y)|_{x=y=1}=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}\frac{d_u d_v}{d_u+d_v}$.

(vi) $(S_yD_x+S_xD_y)MIBSP(H;x,y)=(S_yD_x)(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}x^{d_u}y^{d_v})+(S_xD_y)(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}x^{d_u}y^{d_v})$

$$=S_y(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}d_u x^{d_u}y^{d_v})+S_x(\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}d_v x^{d_u}y^{d_v})$$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}\tfrac{d_u}{d_v}x^{d_u}y^{d_v}+\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}\tfrac{d_v}{d_u}x^{d_u}y^{d_v}$$

$$=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(\tfrac{d_u}{d_v}+\tfrac{d_v}{d_u})x^{d_u}y^{d_v}$$

Since, $d_u=Min\{d_u,d_v\}$ and $d_v=Max\{d_u,d_v\}$

Therefore, $\mathcal{M}\mathrm{SSD}(H)=(S_yD_x+S_xD_y)MIBSP(H;x,y)|_{x=y=1}=\sum_{r=1}^{\alpha}\sum_{\forall uv\in X_r}(\frac{Min\{d_u,d_v\}}{Max\{d_u,d_v\}}+\frac{Max\{d_u,d_v\}}{Min\{d_u,d_v\}})$.

The following Proposition represent the relationship between $TI(H)$ and $\mathcal{M}TI(H)$.

Proposition 1. *Let $TI(H)$ denotes the degree-based topological indices of a graph H, and let $\mathcal{M}TI(H)$ represent the matching degree-based topological indices of H. The relationship between $TI(H)$ and $\mathcal{M}TI(H)$ depends on the type of graph. For instance:*

(i) $TI(P_n)>\mathcal{M}TI(P_n)$ if n is even and $n\geq 4$, and $TI(P_n)<\mathcal{M}TI(P_n)$ if n is odd and $n\geq 5$.

(ii) $TI(K_n)<\mathcal{M}TI(K_n)$, if $n\geq 4$.

(iii) $TI(C_n)=\mathcal{M}TI(C_n)$ if n is even, and $TI(C_n)<\mathcal{M}TI(C_n)$ if n is odd and $n>3$.

Comparing MIBSP to Wiener and Hosoya indices. Results confirm MIBSP's superiority in modeling conjugated systems: its bivariate polynomial captures resonance effects (e.g., bond delocalization) that path-length-based indices (Wiener) or univariate matching counts (Hosoya) cannot detect, solidifying its utility for electronic structure analysis.

3.2. Maximum Independent Bond Set Polynomials of Various Painkillers Drugs Structures

In this subsection, we determine the maximum independent bond set polynomials of various Painkillers drugs structures, such as: Aspirin, Paracetamol, Caffeine, Ibuprofen, Phenacetin and Salicylic acid. Moreover, computing some matching degree-based topological indices such as: Matching First Zagreb index, Matching second Zagreb index,

matching general Randic index, matching Harmonic index, matching inverse sum index and matching Symmetric division degree index related to the maximum independent bonds set polynomial of the chemical structure of such drugs.

The graph derived from the chemical structure of Aspirin has order $|V(H_{Aspirin})| = 13$ and size $|E(H_{Aspirin})| = 13$. In addition the vertices labeled as $v_i, i = 1, 2, ..., 13$.

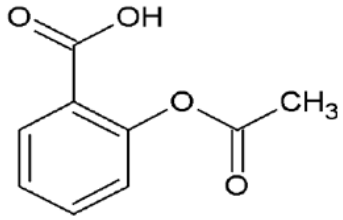

Figure 1: Chemical structure of Aspirin(Acetylsalicylic) drug, adapted from [41].

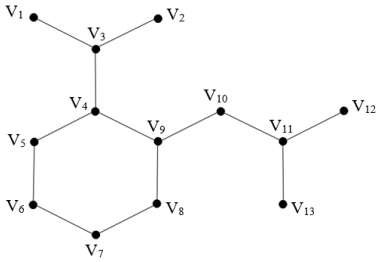

Figure 2: Graph of Aspirin(Acetylsalicylic) drug structure.

The following theorem determines the maximum independent bond set polynomials of the graph representing the structure of the Aspirin drug.

Theorem 2. *Let $H_{Aspirin}$ be a graph of Aspirin drug structure. Then, the maximum independent bond set polynomials is: $MIBSP(H_{Aspirin}) = 46xy^3 + 38x^2y^2 + 38x^2y^3 + 8x^3y^3$.*

Proof. Let $H_{Aspirin}$ be a graph of Aspirin drug structure. Then, the matching number $\beta(H_{Aspirin}) = 5$, this means the maximum independent bond set contains 5 edges and we have 26 maximum matching which are given in the next Table 2.

Table 2: Maximum matching $X_i, i = 1, 2, ..., 26$ of $H_{Aspirin}$ and their M-polynomials

X_i	Maximum matching	$M(X_i; x, y)$
X_1	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}\}$	$xy^3 + x^2y^2 + 3x^2y^3$
X_2	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}\}$	$xy^3 + x^2y^2 + 3x^2y^3$
X_3	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9, v_{11}v_{12}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$

X_4	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9, v_{11}v_{12}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_5	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9, v_{11}v_{13}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_6	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9, v_{11}v_{13}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_7	$\{v_1v_3, v_4v_9, v_7v_8, v_5v_6, v_{10}v_{11}\}$	$xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_8	$\{v_2v_3, v_4v_9, v_7v_8, v_5v_6, v_{10}v_{11}\}$	$xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_9	$\{v_1v_3, v_4v_9, v_7v_8, v_5v_6, v_{11}v_{12}\}$	$2xy^3 + 2x^2y^2 + x^3y^3$
X_{10}	$\{v_2v_3, v_4v_9, v_7v_8, v_5v_6, v_{11}v_{12}\}$	$2xy^3 + 2x^2y^2 + x^3y^3$
X_{11}	$\{v_1v_3, v_4v_9, v_7v_8, v_5v_6, v_{11}v_{13}\}$	$2xy^3 + 2x^2y^2 + x^3y^3$
X_{12}	$\{v_2v_3, v_4v_9, v_7v_8, v_5v_6, v_{11}v_{13}\}$	$2xy^3 + 2x^2y^2 + x^3y^3$
X_{13}	$\{v_1v_3, v_4v_5, v_7v_8, v_9v_{10}, v_{11}v_{12}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{14}	$\{v_2v_3, v_4v_5, v_7v_8, v_9v_{10}, v_{11}v_{12}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{15}	$\{v_1v_3, v_4v_5, v_7v_8, v_9v_{10}, v_{11}v_{13}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{16}	$\{v_2v_3, v_4v_5, v_7v_8, v_9v_{10}, v_{11}v_{13}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{17}	$\{v_1v_3, v_4v_5, v_6v_7, v_9v_{10}, v_{11}v_{12}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{18}	$\{v_2v_3, v_4v_5, v_6v_7, v_9v_{10}, v_{11}v_{12}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{19}	$\{v_1v_3, v_4v_5, v_6v_7, v_9v_{10}, v_{11}v_{13}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{20}	$\{v_2v_3, v_4v_5, v_6v_7, v_9v_{10}, v_{11}v_{13}\}$	$2xy^3 + x^2y^2 + 2x^2y^3$
X_{21}	$\{v_1v_3, v_5v_6, v_7v_8, v_9v_{10}, v_{11}v_{12}\}$	$2xy^3 + 2x^2y^2 + x^2y^3$
X_{22}	$\{v_2v_3, v_5v_6, v_7v_8, v_9v_{10}, v_{11}v_{12}\}$	$2xy^3 + 2x^2y^2 + x^2y^3$
X_{23}	$\{v_1v_3, v_5v_6, v_7v_8, v_9v_{10}, v_{11}v_{13}\}$	$2xy^3 + 2x^2y^2 + x^2y^3$
X_{24}	$\{v_2v_3, v_5v_6, v_7v_8, v_9v_{10}, v_{11}v_{13}\}$	$2xy^3 + 2x^2y^2 + x^2y^3$
X_{25}	$\{v_3v_4, v_5v_6, v_7v_8, v_9v_{10}, v_{11}v_{12}\}$	$xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_{26}	$\{v_3v_4, v_5v_6, v_7v_8, v_9v_{10}, v_{11}v_{13}\}$	$xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$

Thus, for each case of maximum matching we classify the independent edges and obtain the M-polynomial as given in the third column. Finally, we add all M-polynomials in the third column to get the maximum independent bond set polynomials.
$MIBSP(H_{Aspirin}) = 46xy^3 + 38x^2y^2 + 38x^2y^3 + 8x^3y^3$.

Corollary 1. *Let $H_{Aspirin}$ be a graph of Aspirin drug structure. Then,*

(i) $\mathcal{M}M_1(H_{Aspirin}) = 574$.

(ii) $\mathcal{M}M_2(H_{Aspirin}) = 590$.

(iii) $\mathcal{M}R_\gamma(H_{Aspirin}) = 46(3^\gamma) + 38(4^\gamma) + 38(6^\gamma) + 8(9^\gamma)$.

(iv) $\mathcal{M}SSD(H_{Aspirin}) = \frac{983}{3}$.

(v) $\mathcal{M}\mathrm{H}(\mathrm{H_{Aspirin}}) = \frac{898}{15}$.

(vi) $\mathcal{M}\mathrm{I}(\mathrm{H_{Aspirin}}) = \frac{1301}{10}$.

The graph derived from the chemical structure of Paracetamol has order $|V(H_{Paracetamol})| = 11$ and size $|E(H_{Paracetamol})| = 11$. In addition the vertices labeled as $v_i, i = 1, 2, ..., 11$.

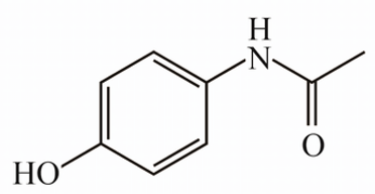

Figure 3: Chemical structure of Paracetamol drug, adapted from [42].

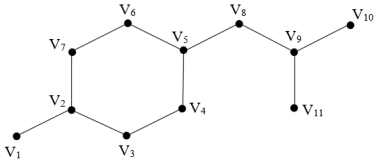

Figure 4: Graph of Paracetamol drug structure.

The following theorem determines the maximum independent bond set polynomials of the graph representing the structure of the Paracetamol drug.

Theorem 3. *Let $H_{Paracetamol}$ be a graph of Paracetamol drug structure. Then, the maximum independent bond set polynomials is: $MIBSP(H_{Paracetamol}) = 4xy^3+4x^2y^2+2x^2y^3$.*

Proof. Let $H_{Paracetamol}$ be a graph of Paracetamol drug structure. Then, the matching number $\beta(H_{Paracetamol}) = 5$, this means the maximum independent bond set contains 5 edges and we have 2 maximum matching which are:
$X_1 = \{v_1v_2, v_3v_4, v_6v_7, v_5v_8, v_9v_{10}\}$ and $X_2 = \{v_1v_2, v_3v_4, v_6v_7, v_5v_8, v_9v_{11}\}$.
Since, $M(X_1; x, y) = M(X_2; x, y) = 2xy^3 + 2x^2y^2 + x^2y^3$.
Hence, $MIBSP(H_{Paracetamol}) = M(X_1; x, y) + M(X_2; x, y) = 4xy^3 + 4x^2y^2 + 2x^2y^3$

Corollary 2. *Let $H_{Paracetamol}$ be a graph of Paracetamol drug structure. Then,*

(i) $\mathcal{M}M_1(H_{Paracetamol}) = 42$.

(ii) $\mathcal{M}M_2(H_{Paracetamol}) = 40$.

(iii) $\mathcal{M}R_\gamma(H_{Paracetamol}) = 4(3^\gamma) + 4(4^\gamma) + 2(6^\gamma)$.

(iv) $\mathcal{M}SSD(H_{Paracetamol}) = \frac{77}{3}$.

(v) $\mathcal{M}\mathrm{H}(\mathrm{H}_{\mathrm{Paracetamol}}) = \frac{24}{5}$.

(vi) $\mathcal{M}\mathrm{I}(\mathrm{H}_{\mathrm{Paracetamol}}) = \frac{47}{5}$.

The graph derived from the chemical structure of Caffeine has order $|V(H_{Caffeine})| = 14$ and size $|E(H_{Caffeine})| = 15$. In addition the vertices labeled as $v_i, i = 1, 2, ..., 14$.

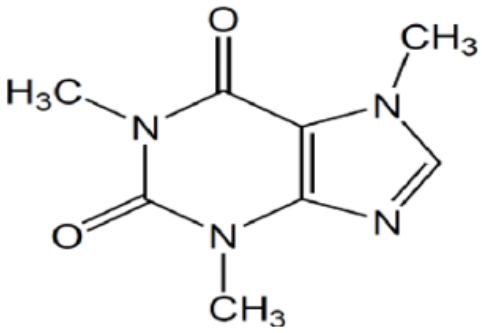

Figure 5: Chemical structure of Caffeine drug, adapted from [43].

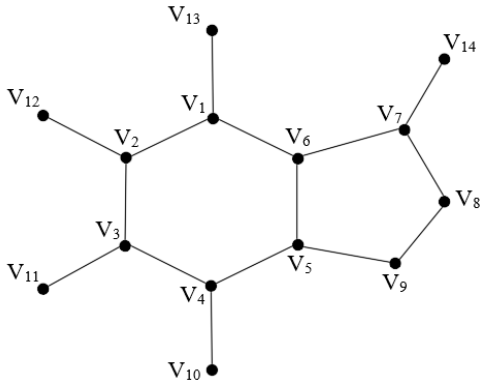

Figure 6: Graph of Caffeine drug structure.

The following theorem determines the maximum independent bond set polynomials of the graph representing the structure of the Caffeine drug.

Theorem 4. *Let $H_{Caffeine}$ be a graph of Caffeine drug structure. Then, the maximum independent bond set polynomials is: $MIBSP(H_{Caffeine}) = 5xy^3 + x^2y^2 + x^3y^3$.*

Proof. Let $H_{Caffeine}$ be a graph of Caffeine drug structure. Then, the matching number $\beta(H_{Caffeine}) = 7$, this means the maximum independent bond set contains 7 edges and we have only one maximum matching which is:
$X = \{v_4v_{10}, v_3v_{11}, v_2v_{12}, v_1v_{13}, v_7v_{14}, v_5v_6, v_8v_9\}$. This matching is called a perfect matching in $H_{Caffeine}$ because every vertex in $V(H_{Caffeine})$ is incident to exactly one edge in X. Since, we have only one maximum matching. Therefore, $MIBSP(H_{Caffeine}) = M(X; x, y) = 5xy^3 + x^2y^2 + x^3y^3$

Corollary 3. *Let $H_{Caffeine}$ be a graph of Caffeine drug structure. Then,*

(i) $\mathcal{M}M_1(H_{Caffeine}) = 30$.

(ii) $\mathcal{M}M_2(H_{Caffeine}) = 28.$

(iii) $\mathcal{M}R_\gamma(H_{Caffeine}) = 5(3^\gamma) + (4^\gamma) + 9^\gamma.$

(iv) $\mathcal{M}SSD(H_{Caffeine}) = \frac{62}{3}.$

(v) $\mathcal{M}\mathrm{H}(\mathrm{H_{Caffeine}}) = \frac{10}{3}.$

(vi) $\mathcal{M}\mathrm{I}(\mathrm{H_{Caffeine}}) = \frac{75}{12}.$

The graph derived from the chemical structure of Ibuprofen has order $|V(H_{Ibuprofen})| = 15$ and size $|E(H_{Ibuprofen})| = 15$. In addition the vertices labeled as $v_i, i = 1, 2, ..., 15$.

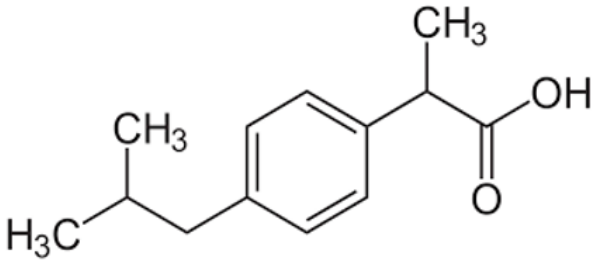

Figure 7: Chemical structure of Ibuprofen drug, adapted from [41].

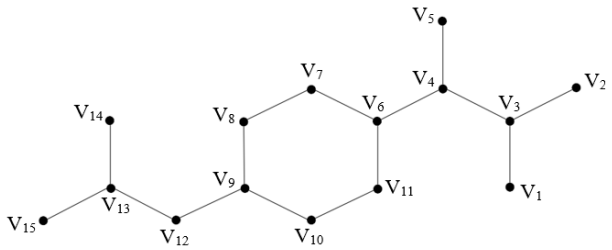

Figure 8: Graph of Ibuprofen drug structure.

The following theorem determines the maximum independent bond set polynomials of the graph representing the structure of the Ibuprofen drug.

Theorem 5. *Let $H_{Ibuprofen}$ be a graph of Ibuprofen drug structure. Then, the maximum independent bond set polynomials is: $MIBSP(H_{Ibuprofen}) = 76xy^3 + 36x^2y^2 + 52x^2y^3 + 4x^3y^3$.*

Proof. Let $H_{Ibuprofen}$ be a graph of Ibuprofen drug structure. Then, the matching number $\beta(H_{Ibuprofen}) = 6$, this means the maximum independent bond set contains 6 edges and we have 28 maximum matching which are given in the next Table 3.

Table 3: Maximum matching $X_i, i = 1, 2, ..., 28$ of $H_{Ibuprofen}$ and their M-polynomials

X_i	Maximum matching	$M(X_i; x, y)$
X_1	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}, v_{12}v_{13}\}$	$2xy^3 + x^2y^2 + 3x^2y^3$
X_2	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}, v_{12}v_{13}\}$	$2xy^3 + x^2y^2 + 3x^2y^3$
X_3	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_4	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_5	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_6	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9, v_{10}v_{11}, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_7	$\{v_1v_3, v_4v_5, v_6v_{11}, v_9v_{10}, v_7v_8, v_{12}v_{13}\}$	$2xy^3 + x^2y^2 + 3x^2y^3$
X_8	$\{v_2v_3, v_4v_5, v_6v_{11}, v_9v_{10}, v_7v_8, v_{12}v_{13}\}$	$2xy^3 + x^2y^2 + 3x^2y^3$
X_9	$\{v_1v_3, v_4v_5, v_6v_{11}, v_9v_{10}, v_7v_8, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{10}	$\{v_2v_3, v_4v_5, v_6v_{11}, v_9v_{10}, v_7v_8, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{11}	$\{v_1v_3, v_4v_5, v_6v_{11}, v_9v_{10}, v_7v_8, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{12}	$\{v_2v_3, v_4v_5, v_6v_{11}, v_9v_{10}, v_7v_8, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{13}	$\{v_1v_3, v_4v_6, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$2xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_{14}	$\{v_2v_3, v_4v_6, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$2xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_{15}	$\{v_1v_3, v_4v_6, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$2xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_{16}	$\{v_2v_3, v_4v_6, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$2xy^3 + 2x^2y^2 + x^2y^3 + x^3y^3$
X_{17}	$\{v_1v_3, v_4v_5, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$3xy^3 + 2x^2y^2 + x^2y^3$
X_{18}	$\{v_2v_3, v_4v_5, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$3xy^3 + 2x^2y^2 + x^2y^3$
X_{19}	$\{v_1v_3, v_4v_5, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$3xy^3 + 2x^2y^2 + x^2y^3$
X_{20}	$\{v_2v_3, v_4v_5, v_7v_8, v_{10}v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$3xy^3 + 2x^2y^2 + x^2y^3$
X_{21}	$\{v_1v_3, v_4v_5, v_6v_7, v_{10}v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{22}	$\{v_2v_3, v_4v_5, v_6v_7, v_{10}v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{23}	$\{v_1v_3, v_4v_5, v_6v_7, v_{10}v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{24}	$\{v_2v_3, v_4v_5, v_6v_7, v_{10}v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{25}	$\{v_1v_3, v_4v_5, v_7v_8, v_6v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{26}	$\{v_2v_3, v_4v_5, v_7v_8, v_6v_{11}, v_9v_{12}, v_{13}v_{15}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{27}	$\{v_1v_3, v_4v_5, v_7v_8, v_6v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$
X_{28}	$\{v_2v_3, v_4v_5, v_7v_8, v_6v_{11}, v_9v_{12}, v_{13}v_{14}\}$	$3xy^3 + x^2y^2 + 2x^2y^3$

Thus, for each case of maximum matching we classify the independent edges and obtain the M-polynomial as given in the third column. Finally, we add all M-polynomials in the third column to get the maximum independent bond set polynomials.
$MIBSP(H_{Ibuprofen}) = 76xy^3 + 36x^2y^2 + 52x^2y^3 + 4x^3y^3$.

Corollary 4. *Let $H_{Ibuprofen}$ be a graph of Ibuprofen drug structure. Then,*

(i) $\mathcal{M}M_1(H_{Ibuprofen}) = 732$.

(ii) $\mathcal{M}M_2(H_{Ibuprofen}) = 720$.

(iii) $\mathcal{M}R_{\gamma}(H_{Ibuprofen}) = 76(3^{\gamma}) + 36(4^{\gamma}) + 52(6^{\gamma}) + 4(9^{\gamma})$.

(iv) $\mathcal{M}SSD(H_{Ibuprofen}) = 446$.

(v) $\mathcal{M}\mathrm{H}(\mathrm{H_{Ibuprofen}}) = \frac{1172}{15}$.

(vi) $\mathcal{M}\mathrm{I}(\mathrm{H_{Ibuprofen}}) = \frac{807}{5}$.

The graph derived from the chemical structure of Phenacetin has the same order and size $|V(H_{Phenacetin})| = |E(H_{Phenacetin})| = 13$. In addition the vertices labeled as $v_i, i = 1, 2, ..., 13$.

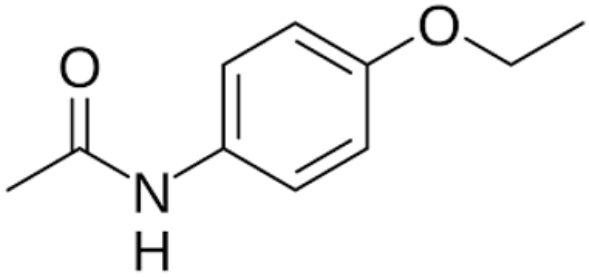

Figure 9: Chemical structure of Phenacetin drug, adapted from [42].

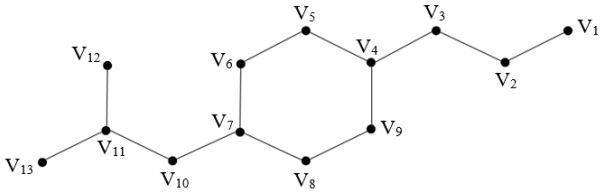

Figure 10: Graph of Phenacetin drug structure.

The following theorem determines the maximum independent bond set polynomials of the graph representing the structure of the Phenacetin drug.

Theorem 6. *Let $H_{Phenacetin}$ be a graph of Phenacetin drug structure. Then, the maximum independent bond set polynomials is: $MIBSP(H_{Phenacetin}) = 2xy^2+2xy^3+4x^2y^2+4x^2y^3$.*

Proof. Let $H_{Phenacetin}$ be a graph of Phenacetin drug structure. Then, the matching number $\beta(H_{Phenacetin}) = 6$, this means the maximum independent bond set contains 6 edges and we have 2 maximum matching which are:
$X_1 = \{v_1v_2, v_3v_4, v_5v_6, v_8v_9, v_7v_{10}, v_{11}v_{12}\}$ and $X_2 = \{v_1v_2, v_3v_4, v_5v_6, v_8v_9, v_7v_{10}, v_{11}v_{13}\}$.
Since, $M(X_1; x, y) = M(X_2; x, y) = xy^2 + xy^3 + 2x^2y^2 + 2x^2y^3$.
Therefore, $MIBSP(H_{Phenacetin}) = M(X_1; x, y) + M(X_2; x, y) = 2xy^2 + 2xy^3 + 4x^2y^2 + 4x^2y^3$.

Corollary 5. *Let $H_{Phenacetin}$ be a graph of Phenacetin drug structure. Then,*

(i) $\mathcal{M}M_1(H_{Phenacetin}) = 50.$

(ii) $\mathcal{M}M_2(H_{Phenacetin}) = 50.$

(iii) $\mathcal{M}R_\gamma(H_{Phenacetin}) = 2(2^\gamma) + 2(3^\gamma) + 4(4^\gamma) + 4(6^\gamma).$

(iv) $\mathcal{M}SSD(H_{Phenacetin}) = \frac{85}{3}.$

(v) $\mathcal{M}\mathrm{H}(\mathrm{H}_{\mathrm{Phenacetin}}) = \frac{89}{15}.$

(vi) $\mathcal{M}\mathrm{I}(\mathrm{H}_{\mathrm{Phenacetin}}) = \frac{349}{30}.$

The graph derived from the chemical structure of Salicylic acid also has the same order and size $|V(H_{Salicylicacid})| = |E(H_{Salicylicacid})| = 10$. In addition the vertices labeled as $v_i, i = 1, 2, ..., 10$.

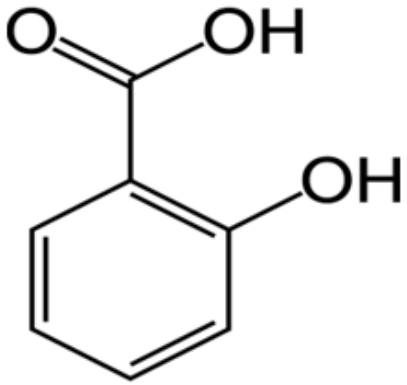

Figure 11: Chemical structure of Salicylic acid drug, adapted from [44].

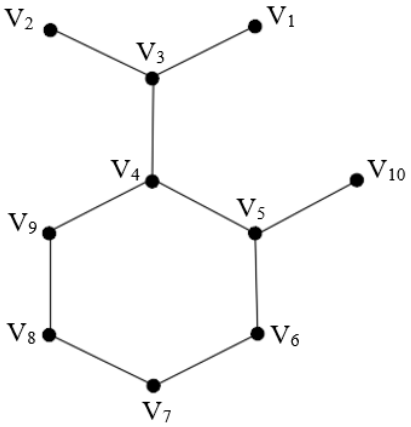

Figure 12: Graph of Salicylic acid drug structure.

The following theorem determines the maximum independent bond set polynomials of the graph representing the structure of the Salicylic acid drug.

Theorem 7. *Let $H_{Salicylicacid}$ be a graph of Salicylic acid drug structure. Then, the maximum independent bond set polynomials is: $MIBSP(H_{Salicylicacid}) = 17xy^3+16x^2y^2+8x^2y^3+3x^3y^3$.*

Proof. Let $H_{Salicylicacid}$ be a graph of Salicylic acid drug structure. Then, the matching number $\beta(H_{Salicylicacid}) = 4$, this means the maximum independent bond set contains 4 edges and we have 11 maximum matching which are given in the next Table 4.

Table 4: Maximum matching $X_i, i = 1, 2, ..., 11$ of $H_{Salicylicacid}$ and their M-polynomials

X_i	Maximum matching	$M(X_i; x, y)$
X_1	$\{v_1v_3, v_4v_5, v_6v_7, v_8v_9\}$	$xy^3 + 2x^2y^2 + x^3y^3$
X_2	$\{v_2v_3, v_4v_5, v_6v_7, v_8v_9\}$	$xy^3 + 2x^2y^2 + x^3y^3$
X_3	$\{v_1v_3, v_5v_6, v_7v_8, v_4v_9\}$	$xy^3 + x^2y^2 + 2x^2y^3$
X_4	$\{v_2v_3, v_5v_6, v_7v_8, v_4v_9\}$	$xy^3 + x^2y^2 + 2x^2y^3$
X_5	$\{v_1v_3, v_4v_9, v_7v_8, v_5v_{10}\}$	$2xy^3 + x^2y^2 + x^2y^3$
X_6	$\{v_2v_3, v_4v_9, v_7v_8, v_5v_{10}\}$	$2xy^3 + x^2y^2 + x^2y^3$
X_7	$\{v_1v_3, v_4v_9, v_6v_7, v_5v_{10}\}$	$2xy^3 + x^2y^2 + x^2y^3$
X_8	$\{v_2v_3, v_4v_9, v_6v_7, v_5v_{10}\}$	$2xy^3 + x^2y^2 + x^2y^3$
X_9	$\{v_1v_3, v_8v_9, v_6v_7, v_5v_{10}\}$	$2xy^3 + 2x^2y^2$
X_{10}	$\{v_2v_3, v_8v_9, v_6v_7, v_5v_{10}\}$	$2xy^3 + 2x^2y^2$
X_{11}	$\{v_3v_4, v_8v_9, v_6v_7, v_5v_{10}\}$	$xy^3 + 2x^2y^2 + x^3y^3$

Thus, for each case of maximum matching we classify the independent edges and obtain the M-polynomial as given in the third column. Finally, we add all M-polynomials in the third column to get the maximum independent bond set polynomials.
$MIBSP(H_{Salicylicacid}) = 17xy^3 + 16x^2y^2 + 8x^2y^3 + 3x^3y^3$.

Corollary 6. *Let $H_{Salicylicacid}$ be a graph of Salicylic acid drug structure. Then,*

(i) $\mathcal{M}M_1(H_{Salicylicacid}) = 190$.

(ii) $\mathcal{M}M_2(H_{Salicylicacid}) = 190$.

(iii) $\mathcal{M}R_\gamma(H_{Salicylicacid}) = 17(3^\gamma) + 16(4^\gamma) + 8(6^\gamma) + 3(9^\gamma)$.

(iv) $\mathcal{M}SSD(H_{Salicylicacid}) = 112$.

(v) $\mathcal{M}\mathrm{H}(\mathrm{H}_{\mathrm{Salicylicacid}}) = \frac{207}{10}$.

(vi) $\mathcal{M}\mathrm{I}(\mathrm{H}_{\mathrm{Salicylicacid}}) = \frac{857}{20}$.

4. Conclusions

Unlike distance-based resolvers (Wiener [18]), MIBSP specializes in electronic structure analysis through degree-weighted matchings. This approach enables the detection of stability variations in conjugated systems such as the perfect matching in Caffeine that remain undetectable via path-length analysis. In this study, we introduced the concept of the maximum independent bond set polynomial $MIBSP(H; x, y)$ and applied it to derive degree-based topological indices for the chemical graphs of several painkiller molecules, including Aspirin, Paracetamol, Caffeine, Ibuprofen, Phenacetin, and Salicylic acid. Our analysis revealed that molecules with a higher number of perfect matchings, such as Caffeine, tend to exhibit more stable and well organized bonding structures, while those with fewer perfect matchings show weaker bonding arrangements, as highlighted in [45]. These findings offer valuable insights into the molecular stability of painkiller compounds and present useful tools for the design of more stable pharmaceutical molecules. Looking ahead, my future research will focus on leveraging the MIBSP-polynomial to identify promising drug candidates with optimal therapeutic properties.

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