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A NEW VARIANT OF THE SOMBOR MATRIX: BOUNDS ON SPECTRAL RADIUS AND ENERGY WITH APPLICATIONS TO QSPR ANALYSIS OF COVID-19 DRUGS

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Abstract. In this paper, we introduce a novel variant of the Sombor matrix, denoted as $\mathcal{NS}o(\zeta)$, for a simple graph $\zeta(\mathcal{V},\mathcal{E})$. The matrix is defined such that for $i \neq j$, the (i,j)-entry is given by $\sqrt{d_i^2 + d_j^2}$, where d_i represents the degree of the i^{th} vertex, and zero otherwise. Let $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_\rho$ denote the eigenvalues of $\mathcal{NS}o(\zeta)$, with η_1 being the spectral radius. The Sombor energy $E_{\mathcal{NS}o}(\zeta)$ is defined as the sum of the absolute values of these eigenvalues. We derive upper and lower bounds for both η_1 and $E_{\mathcal{NS}o}(\zeta)$ in terms of the first Zagreb index $(M_1(\zeta))$. As an application, we perform a Quantitative Structure-Property Relationship (QSPR) analysis using a dataset of drugs employed in the treatment of COVID-19 patients. We construct linear, quadratic, and cubic regression models to explore the relationship between the physicochemical properties of these drugs and their corresponding $E_{\mathcal{NS}o}(\zeta)$ values, with the models visualized through graphical representations.

1. Introduction

Let $\zeta(\mathcal{V},\mathcal{E})$ be a simple graph, with $|\mathcal{V}| = \rho$ and $|\mathcal{E}| = \varrho$. The degree of a vertex $v \in \mathcal{V}$ is the count of edges connected to v denoted by $d_\zeta(v)$. The maximum(minimum) vertex and edge degree of a graph is denoted by $\Delta(\delta)$ and $\Delta'(\delta')$ respectively. A graph ζ is said to be complete if $\Delta = \delta = \rho - 1$ denoted by K_ρ. If a vertex set of a graph ζ is partitioned into two sets say $|\mathcal{M}| = \upsilon$ and $|\mathcal{N}| = \nu$ (partite sets) such that every edge meet both $\mathcal{M}$ and $\mathcal{N}$ then the graph is bipartite graph. If every vertex of $\mathcal{M}$ is adjacent to every vertex of $\mathcal{N}$ then the graph is complete bipartite graph denoted as $K_{\upsilon,\nu}$. The graph $K_{1,\rho-1}$ is called as star graph denoted by $\mathcal{S}_\rho$ and the graph $K_{\nu,\nu}$ is called equi-bipartite graph. The complement of a graph ζ denoted by $\overline{\zeta}$ is a graph defined on same vertex set as of ζ such that if two vertices are adjacent in $\overline{\zeta}$, then they are not adjacent in ζ. For more terminologies refer the following [10].

The first degree-based molecular descriptor, the Zagreb index, was developed by Gutman and Trinajstić [9]. It firstly emerged in the topological formula for conjugated molecules regarding their total π-electron energy. The first Zagreb index is defined as:

$$M_1(\zeta) = \sum_{v \in V(\zeta)} d_\zeta(v)^2 = \sum_{e=uv \in E(\zeta)} (d_\zeta(u) + d_\zeta(v)) \tag{1.1}$$

There is another topological index which is widely known and used in applications of graph theory specially in Chemistry. The Sombor index [7] is given by

$$SO(\zeta) = \sum_{e=uv \in E(\zeta)} \sqrt{d_\zeta(u)^2 + d_\zeta(v)^2} \tag{1.2}$$

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A square matrix $\mathcal{A}(\zeta)$ of order ρ is an adjacency matrix of ζ whose (i,j)-entry is 1 if the vertex v_i is adjacent to v_j, and is 0 otherwise. The energy $E(\zeta)$ of a graph ζ is the sum of the absolute values of eigenvalues of $\mathcal{A}(\zeta)$. This quantity is introduced in [8]. Suppose $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_\rho$ are the eigenvalues of the adjacency matrix $\mathcal{A}(\zeta)$ then the energy of the graph ζ is given by

$$E = E(\zeta) = \sum_{i=1}^{\rho} |\lambda_i| \tag{1.3}$$

Sumedha S. Shinde et al. [18] proposed a Sombor matrix for a graph ζ, denoted as $SOM(\zeta)$, further obtained bounds for its eigenvalues and Sombor energy. Let $\mu_1 \geq \mu_2 \geq ... \geq \mu_n$ and $E_{SOM}(\zeta)$ be the eigenvalues and Sombor energy of $SOM(\zeta)$.

Here we define a new variant of Sombor matrix $\mathcal{NS}o(\zeta)$ as

$$\mathcal{NS}o(\zeta) = \begin{cases} \sqrt{d_i^2 + d_j^2}, & \text{if } i \neq j \\ 0, & \text{otherwise} \end{cases}$$

where d_i represents the degree of the i^{th}vertex. The characteristic polynomial for $\mathcal{NS}o(\zeta)$ is defined as $\psi(\zeta,\eta) = det(\eta I - \mathcal{NS}o(\zeta)) = |\eta I - \mathcal{NS}o(\zeta)| = \eta^\rho + r_1\eta^{\rho-1} + ... + r_\rho = 0$, here I represents the identity matrix of order ρ. Since $\mathcal{NS}o(\zeta)$ is a real symmetric matrix, the roots of $\psi(\zeta,\eta) = 0$ are real and it can written in descending order as $\eta_1 \geq \eta_2 \geq ... \geq \eta_\rho$, with respective multiplicities $\tau_1, \tau_2, ..., \tau_\rho$ then the spectrum can be written as,

$$Spectra(\mathcal{NS}o(\zeta)) = \begin{pmatrix} \eta_1 & \eta_2 & \cdots & \eta_\rho \\ \tau_1 & \tau_2 & \cdots & \tau_\rho \end{pmatrix}$$

where η_1 is the spectral radius. Sombor energy of ζ is given as,

$$E_{\mathcal{NS}o}(\zeta) = \sum_{i=1}^{\rho} |\eta_i| \tag{1.4}$$

For more studies on graph energy refer [1, 2, 16, 17].

Remark 1.1. The Sombor matrix $SOM(\zeta)$ and energy is defined in [18], we try to relate the newly variant Sombor matrix $\mathcal{NS}o(\zeta)$ with $SOM(\zeta)$. The matrix and eigenvalues of the matrix are equal if and only if $\zeta = K_\rho$ or $\zeta = \overline{K_\rho}$. Further the energy of $\mathcal{NS}o(\zeta) = 2\eta_1$ (η_1 being the spectral radius) for any graph G, which is not the same in the case of energy of $SOM(\zeta)$. The energy of $SOM(\zeta)$ is always less then or equal to $\mathcal{NS}o(\zeta)$ for any graph ζ.

2. Preliminaries

Lemma 2.1. [4] *(Cauchy Schwartz inequality) Let a_i and b_i, $1 \leq i \leq n$ be any real numbers, then*

$$\left(\sum_{i=1}^{\rho} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{\rho} a_i^2\right)\left(\sum_{i=1}^{\rho} b_i^2\right). \tag{2.1}$$

Lemma 2.2. [11] *Let a_i, $1 \leq i \leq n$ be any real numbers, then*

$$\left(\sum_{i=1}^{\rho} |a_i|\right)^2 \geq \left(\sum_{i=1}^{\rho} |a_i|^2\right). \tag{2.2}$$

Lemma 2.3. [13] *(Ozeki inequality) If a_i and b_i $(1 \leq i \leq n)$ are non-negative real numbers then*

$$\sum_{i=1}^{\rho} a_i^2 \sum_{i=1}^{\rho} b_i^2 - \left[\sum_{i=1}^{\rho} a_i b_i\right]^2 \leq \frac{n^2}{4}\left(M_1 M_2 - m_1 m_2\right)^2, \tag{2.3}$$

where $M_1 = max_{1\leq i\leq n}\{a_i\}$, $M_2 = max_{1\leq i\leq n}\{b_i\}$, $m_1 = min_{1\leq i\leq n}\{a_i\}$, $m_2 = min_{1\leq i\leq n}\{b_i\}$.

Lemma 2.4. [15] *Suppose* a_i *and* b_i, $1 \leq i \leq n$ *are positive real numbers, then*

$$\sum_{i=1}^{\rho} a_i^2 \sum_{i=1}^{\rho} b_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{\rho} a_ib_i\right)^2, \tag{2.4}$$

where $M_1 = max_{1\leq i\leq n}\{a_i\}$, $M_2 = max_{1\leq i\leq n}\{b_i\}$, $m_1 = min_{1\leq i\leq n}\{a_i\}$, $m_2 = min_{1\leq i\leq n}\{b_i\}$.

Lemma 2.5. [3] *Suppose* a_i *and* b_i, $1 \leq i \leq n$ *are positive real numbers, then*

$$\left| n\sum_{i=1}^{\rho} a_ib_i - \sum_{i=1}^{\rho} a_i \sum_{i=1}^{\rho} b_i \right| \leq \alpha(n)(A-a)(B-b), \tag{2.5}$$

where a, b, A *and* B *are real constants, that for each* i, $1 \leq i \leq n$, $a \leq a_i \leq A$ *and* $b \leq b_i \leq B$*; further,*

$$\alpha(n) = n\lfloor\frac{n}{2}\rfloor\left(1 - \frac{1}{n}\lfloor\frac{n}{2}\rfloor\right).$$

Lemma 2.6. [5] *Let* a_i *and* b_i, $1 \leq i \leq n$ *are non-negative real numbers, then*

$$\sum_{i=1}^{\rho} b_i^2 + rR\sum_{i=1}^{\rho} a_i^2 \leq (r+R)\left(\sum_{i=1}^{\rho} a_ib_i\right), \tag{2.6}$$

where r *and* R *are real constants, so that for each* i, $1 \leq i \leq n$, *holds,* $ra_i \leq b_i \leq Ra_i$.

Lemma 2.7. [12] *Let* $a_1 \geq a_2 \geq \cdots \geq a_n \geq 0$ *be a sequence of non-negative real numbers. Then*

$$\sum_{i=1}^{\rho} a_i + n(\rho-1)\left(\prod_{i=1}^{\rho} a_i\right)^{1/\rho} \leq \left[\sum_{i=1}^{\rho}\sqrt{a_i}\right]^2 \leq (\rho-1)\sum_{i=1}^{\rho} a_i + n\left(\prod_{i=1}^{\rho} a_i\right)^{1/\rho}. \tag{2.7}$$

Lemma 2.8. [6] *Let* a_i, b_i, c_i *and* d_i *are sequences of real numbers and* p_i, q_i *are non-negative for* $i = 1, 2, ..., n$. *Then the following inequality is valid*

$$\sum_{i=1}^{\rho} p_ia_i^2 \sum_{i=1}^{\rho} q_ib_i^2 + \sum_{i=1}^{\rho} p_ic_i^2 \sum_{i=1}^{\rho} q_id_i^2 \geq 2\sum_{i=1}^{\rho} p_ia_ic_i \sum_{i=1}^{\rho} q_ib_id_i. \tag{2.8}$$

3. Main Results

Lemma 3.1. *Consider a simple connected graph* ζ *with* d_i *representing the degree of the* i^{th} *vertex. Let* $\mathcal{NS}o(\zeta)$ *be a new variant Sombor matrix of the graph* ζ *with eigenvalues* $\eta_1 \geq \eta_2 \geq ... \geq \eta_\rho$, *then*

$$\sum_{i=1}^{\rho} \eta_i^2 = 2(\rho-1)M_1(G).$$

Proof. Indeed, we can calculate as below:

$$\begin{aligned}
\sum_{i=1}^{\rho} \eta_i^2 &= trace([\mathcal{NS}o(\zeta)]^2) \\
&= \sum_{i=1}^{\rho}\sum_{j=1}^{\rho} d_{ij}d_{ji} \\
&= \sum_{i=1}^{\rho}\sum_{j=1}^{\rho} d_{ij}^2 \\
&= 2\sum_{i<j}\left(\sqrt{d_i^2+d_j^2}\right)^2 \\
&= 2\sum_{i<j}(d_i^2+d_j^2) \\
&= 2(\rho-1)M_1(G),
\end{aligned}$$

where we have used

$$\sum_{i<j}(d_i^2+d_j^2) = (\rho-1)M_1(\zeta).$$

□

3.1. Some bounds on spectral radius (η_1) and $E_{\mathcal{NS}o(\zeta)}$ of a new variant of Sombor matrix of a graph.

Theorem 3.2. *Let ζ be a connected graph with ρ vertices and η_1 be the spectral radius (the largest eigenvalue), then*

$$\eta_1 \leq \sqrt{\frac{2(\rho-1)^2M_1(\zeta)}{\rho}}. \tag{3.1}$$

Proof. Since $\sum_{i=1}^{\rho}\eta_i = 0$, it can be rewritten as $\sum_{i=2}^{\rho}\eta_i = -\eta_1$. Further $\left(\sum_{i=1}^{\rho}(\eta_i)^2\right) = 2(\rho-1)M_1(\zeta)$, $\left(\sum_{i=2}^{\rho}(\eta_i)^2\right) = \left(\sum_{i=1}^{\rho}(\eta_i)^2-(\eta_1)^2\right) = \big(2(\rho-1)M_1(\zeta)-(\eta_1)^2\big)$ and $\left(\sum_{i=2}^{\rho}1\right) = (\rho-1)$.

Substituting $a_i = 1$ and $b_i = \eta_i$ in Lemma 2.1 we get

$$\begin{aligned}
(-\eta_1)^2 &\leq (\rho-1)(2(\rho-1)M_1(\zeta)-(\eta_1)^2) \\
&\leq 2(\rho-1)^2M_1(\zeta)-(\rho-1)(\eta_1)^2 \\
&\leq 2(\rho-1)^2M_1(\zeta)-\rho(\eta_1)^2+(\eta_1)^2; \\
\rho(\eta_1)^2 &\leq 2(\rho-1)^2M_1(\zeta); \\
\eta_1 &\leq \sqrt{\frac{2(\rho-1)^2M_1(\zeta)}{\rho}}.
\end{aligned}$$

This completes the proof. □

Theorem 3.3. *Let ζ be a connected graph with ρ vertices, then*

$$\sqrt{2(\rho-1)M_1(\zeta)} \leq E_{\mathcal{NS}o(\zeta)} \leq \sqrt{2\rho(\rho-1)M_1(\zeta)}. \tag{3.2}$$

Proof. Note that

$$E_{\mathcal{NS}o(\zeta)} = \sum_{i=1}^{\rho} |\eta_i|, \quad \sum_{i=1}^{\rho} 1 = \rho, \quad \text{and} \quad \sum_{i=1}^{\rho} |\eta_i|^2 = 2(\rho-1)M_1(\zeta). \tag{3.3}$$

Substituting $a_i = |\eta_i|$ and $b_i = 1$ in Lemma 2.1, we get

$$\begin{aligned} E^2_{\mathcal{NS}o(\zeta)} &\leq 2(\rho-1)M_1(\zeta)\rho, \\ E_{\mathcal{NS}o(\zeta)} &\leq \sqrt{2\rho(\rho-1)M_1(\zeta)}. \end{aligned}$$

Also, substituting $a_i = |\eta_i|$ in Lemma 2.2, we get

$$\begin{aligned} E^2_{\mathcal{NS}o(\zeta)} &\geq 2(\rho-1)M_1(\zeta), \\ E_{\mathcal{NS}o(\zeta)} &\geq \sqrt{2(\rho-1)M_1(\zeta)}. \end{aligned}$$

This gives us both the upper and lower bounds. This completes the proof. □

Theorem 3.4. *Let ζ be a connected graph with ρ vertices. Then*

$$E_{\mathcal{NS}o(\zeta)} \geq \frac{2\sqrt{2(\rho-1)M_1(\zeta)|\eta_1||\eta_\rho|}}{|\eta_1| + |\eta_\rho|}. \tag{3.4}$$

Proof. Let $|\eta_1|$ and $|\eta_\rho|$ be the largest and the smallest eigenvalues. By (3.3) and substituting $a_i = |\eta_i|$, $b_i = 1$, $M_1 = |\eta_1|$, $m_1 = |\eta_\rho|$, $M_2 = 1$ and $m_2 = 1$ in Lemma 2.4, we get

$$\begin{aligned} \sum_{i=1}^{\rho} |\eta_i|^2 \sum_{i=1}^{\rho} 1 &\leq \frac{1}{4}\left(\sqrt{\frac{|\eta_1|}{|\eta_\rho|}} + \sqrt{\frac{|\eta_\rho|}{|\eta_1|}}\right)^2 \left(\sum_{i=1}^{\rho} |\eta_i|\right)^2, \\ 2(\rho-1)M_1(\zeta)\rho &\leq \frac{1}{4}\left(\frac{(|\eta_1| + |\eta_\rho|)}{\sqrt{|\eta_\rho||\eta_1|}}\right)^2 E^2_{\mathcal{NS}o(\zeta)}, \\ 2\rho(\rho-1)M_1(\zeta) &\leq \frac{1}{4}\left(\frac{(|\eta_1| + |\eta_\rho|)^2}{|\eta_\rho||\eta_1|}\right) E^2_{\mathcal{NS}o(\zeta)}, \\ \frac{8\rho(\rho-1)M_1(\zeta)|\eta_\rho||\eta_1|}{(|\eta_1| + |\eta_n|)^2} &\leq E^2_{\mathcal{NS}o(\zeta)}, \\ E_{\mathcal{NS}o(\zeta)} &\geq \sqrt{\frac{8\rho(\rho-1)M_1(\zeta)|\eta_1||\eta_\rho|}{(|\eta_1| + |\eta_\rho|)^2}}, \\ E_{\mathcal{NS}o(\zeta)} &\geq \frac{2\sqrt{2\rho(\rho-1)M_1(\zeta)|\eta_1||\eta_\rho|}}{|\eta_1| + |\eta_\rho|}. \end{aligned}$$

This completes the proof. □

Theorem 3.5. *Let ζ be a connected graph with ρ vertices. Then*

$$E_{\mathcal{NS}o(\zeta)} \geq \frac{\sqrt{8\rho(\rho-1)M_1(\zeta) - \rho^2(|\eta_1| - |\eta_\rho|)^2}}{2}. \tag{3.5}$$

Proof. Let $|\eta_1|$ and $|\eta_\rho|$ be the largest and the smallest eigenvalues. By (3.3) and substituting $a_i = |\eta_i|$, $b_i = 1$, $M_1 = |\eta_1|$, $m_1 = |\eta_\rho|$, $M_2 = 1$ and $m_2 = 1$ in Lemma 2.3, we get

$$\begin{aligned}
\sum_{i=1}^{\rho}|\eta_i|^2\sum_{i=1}^{\rho}1-\left(\sum_{i=1}^{\rho}|\eta_i|\right)^2 &\leq \frac{\rho^2}{4}(|\eta_1|-|\eta_\rho|)^2,\\
2(\rho-1)M_1(\zeta)\rho - E^2_{\mathcal{NS}o(\zeta)} &\leq \frac{\rho^2}{4}(|\eta_1|-|\eta_\rho|)^2,\\
2\rho(\rho-1)M_1(\zeta)-\frac{\rho^2}{4}(|\eta_1|-|\eta_\rho|)^2 &\leq E^2_{\mathcal{NS}o(\zeta)},\\
\frac{8\rho(\rho-1)M_1(\zeta)-\rho^2(|\eta_1|-|\eta_\rho|)^2}{4} &\leq E^2_{\mathcal{NS}o(\zeta)},\\
E_{\mathcal{NS}o(\zeta)} &\geq \frac{\sqrt{8\rho(\rho-1)M_1(\zeta)-\rho^2(|\eta_1|-|\eta_\rho|)^2}}{2}.
\end{aligned}$$

This completes the proof. □

Theorem 3.6. *Let ζ be a connected graph with ρ vertices. Then*

$$E_{\mathcal{NS}o(\zeta)} \leq |\eta_1| + \sqrt{(2(\rho-1)M_1(\zeta)-|\eta_1|^2)(\rho-1)}. \tag{3.6}$$

Proof. Let $|\eta_1|$ be the largest eigenvalue. Since $E_{\mathcal{NS}o(\zeta)} = \sum_{i=1}^{\rho}|\eta_i|$, we have

$$E_{\mathcal{NS}o(\zeta)} - |\eta_1| = \sum_{i=2}^{\rho}|\eta_i|.$$

Squaring both sides of the above equation and then applying Lemma 2.1, we get

$$\begin{aligned}
(E_{\mathcal{NS}o(\zeta)} - |\eta_1|)^2 &= \left(\sum_{i=2}^{\rho}|\eta_i|\right)^2,\\
(E_{\mathcal{NS}o(\zeta)} - |\eta_1|)^2 = \left(\sum_{i=2}^{\rho}|\eta_i|\cdot 1\right)^2 &\leq \left(\sum_{i=2}^{\rho}|\eta_i|^2\right)\left(\sum_{i=2}^{\rho}1^2\right),\\
(E_{\mathcal{NS}o(\zeta)} - |\eta_1|)^2 &\leq \left(2(\rho-1)M_1(\zeta)-|\eta_1|^2\right)(\rho-1),\\
(E_{\mathcal{NS}o(\zeta)} - |\eta_1|) &\leq \sqrt{\left(2(\rho-1)M_1(\zeta)-|\eta_1|^2\right)(\rho-1)},\\
E_{\mathcal{NS}o(\zeta)} &\leq |\eta_1| + \sqrt{\left(2(\rho-1)M_1(\zeta)-|\eta_1|^2\right)(\rho-1)}.
\end{aligned}$$

This completes the proof. □

Theorem 3.7. *Let ζ be a connected graph with ρ vertices. Then*

$$\begin{aligned}
\sqrt{2(\rho-1)M_1(\zeta)+\rho(\rho-1)[det(\mathcal{NS}o(\zeta))]^{2/\rho}} &\leq \left(E_{\mathcal{NS}o(\zeta)}\right)\\
&\leq \sqrt{2(\rho-1)^2M_1(\zeta)+\rho[det(\mathcal{NS}o(\zeta))]^{2/\rho}}.
\end{aligned}$$

Proof. Since $E_{\mathcal{NS}o(\zeta)} = \sum_{i=1}^{\rho} |\eta_i|$, substituting $a_i = \eta_i^2$ in Lemma 2.7, we get

$$\begin{aligned}
\sum_{i=1}^{\rho} \eta_i^2 + n(\rho-1)\left(\prod_{i=1}^{\rho} \eta_i^2\right)^{1/n} &\leq \left(\sum_{i=2}^{\rho} \sqrt{\eta_i^2}\right)^2 \leq (\rho-1)\sum_{i=1}^{\rho} \eta_i^2 + n\left(\prod_{i=1}^{\rho} \eta_i^2\right)^{1/n}, \\
2(\rho-1)M_1(\zeta) + n(\rho-1)[det(\mathcal{NS}o(\zeta))]^{2/n} &\leq \left(E_{\mathcal{NS}o(\zeta)}\right)^2, \\
&\leq (\rho-1)2(\rho-1)M_1(\zeta) + n[det(\mathcal{NS}o(\zeta))]^{2/n}, \\
2(\rho-1)M_1(\zeta) + n(\rho-1)[det(\mathcal{NS}o(\zeta))]^{2/n} &\leq \left(E_{\mathcal{NS}o(\zeta)}\right)^2, \\
&\leq 2(\rho-1)^2 M_1(\zeta) + n[det(\mathcal{NS}o(\zeta))]^{2/n} \\
\sqrt{2(\rho-1)M_1(\zeta) + n(\rho-1)[det(\mathcal{NS}o(\zeta))]^{2/n}} &\leq \left(E_{\mathcal{NS}o(\zeta)}\right), \\
&\leq \sqrt{2(\rho-1)^2 M_1(\zeta) + n[det(\mathcal{NS}o(\zeta))]^{2/n}}.
\end{aligned}$$

This completes the proof. □

Theorem 3.8. *Let ζ be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. Then*

$$E_{\mathcal{NS}o}(\zeta) \geq \sqrt{2n(\rho-1)M_1(\zeta) - \alpha(n)(|\eta_1| - |\eta_n|)^2}, \tag{3.7}$$

where

$$\alpha(n) = n\lfloor \frac{n}{2} \rfloor \left(1 - \frac{1}{n}\lfloor \frac{n}{2} \rfloor\right).$$

Proof. Let $|\eta_1| \geq |\eta_2| \geq \ldots \geq |\eta_n|$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. By putting $a_i = |\eta_i| = b_i$, $A = |\eta_1| = B$ and $a = |\eta_n| = b$ in Lemma 2.5, we get

$$\begin{aligned}
\left| n\sum_{i=1}^{\rho} |\eta_i|^2 - \left(\sum_{i=1}^{\rho} |\eta_i|\right)^2 \right| &\leq \alpha(n)\left(|\eta_1| - |\eta_n|\right)^2, \\
\left|2n(\rho-1)M_1(\zeta) - (E_{\mathcal{NS}o}(\zeta))^2\right| &\leq \alpha(n)\left(|\eta_1| - |\eta_n|\right)^2, \\
2n(\rho-1)M_1(\zeta) - \alpha(n)(|\eta_1| - |\eta_n|)^2 &\leq (E_{\mathcal{NS}o}(\zeta))^2 \\
E_{\mathcal{NS}o}(\zeta) &\geq \sqrt{2n(\rho-1)M_1(\zeta) - \alpha(n)(|\eta_1| - |\eta_n|)^2}.
\end{aligned}$$

This completes the proof. □

Theorem 3.9. *Let ζ be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. Then*

$$E_{\mathcal{NS}o}(\zeta) \geq \frac{n + 2(\rho-1)M_1(\zeta)(\eta_n\eta_1)}{\eta_n + \eta_1}. \tag{3.8}$$

Proof. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. By putting $a_i = |\eta_i|$, $b_i = 1$, $r = \eta_n$ and $R = \eta_1$, in Lemma 2.6, we get

$$\begin{aligned}
\sum_{i=1}^{\rho} 1^2 + \eta_n\eta_1 \sum_{i=1}^{\rho} |\eta_i|^2 &\leq (\eta_n + \eta_1)\left(\sum_{i=1}^{\rho} |\eta_i|\right), \\
n + 2(\rho-1)M_1(\zeta)(\eta_n\eta_1) &\leq (\eta_n + \eta_1)E_{\mathcal{NS}o}(\zeta), \\
E_{\mathcal{NS}o}(\zeta) &\geq \frac{n + 2(\rho-1)M_1(\zeta)(\eta_n\eta_1)}{\eta_n + \eta_1}.
\end{aligned}$$

This completes the proof. □

Theorem 3.10. *Let ζ be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq ... \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. Then*

$$E_{\mathcal{NS}o}(\zeta) \geq \frac{2(\rho-1)M_1(\zeta)+n\eta_1\eta_n}{\eta_1+\eta_n}. \tag{3.9}$$

Proof. Let $\eta_1 \geq \eta_2 \geq ... \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. By putting $a_i = 1$, $b_i = |\eta_i|$, $r = \eta_n$ and $R = \eta_1$, in Lemma 2.6, we get

$$\begin{aligned}
\sum_{i=1}^{\rho}|\eta_i|^2 + \eta_n\eta_1\sum_{i=1}^{\rho}1^2 &\leq (\eta_n+\eta_1)\left(\sum_{i=1}^{\rho}|\eta_i|\right),\\
2(\rho-1)M_1(\zeta)+n(\eta_n\eta_1) &\leq (\eta_n+\eta_1)E_{\mathcal{NS}o}(\zeta),\\
E_{\mathcal{NS}o}(\zeta) &\geq \frac{2(\rho-1)M_1(\zeta)+n\eta_1\eta_n}{\eta_1+\eta_n}.
\end{aligned}$$

This completes the proof. □

Theorem 3.11. *Let ζ be a non-empty graph with n vertices. Then*

$$E_{\mathcal{NS}o}(\zeta) \leq \sqrt{2((\rho-1)M_1(\zeta))^2+\frac{n^2}{2}}. \tag{3.10}$$

Proof. Let $\eta_1 \geq \eta_2 \geq ... \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(\zeta)$. Substituting $a_i = |\eta_i| = b_i$ and $c_i = d_i = p_i = q_i = 1$ in Lemma 2.8, we get

$$\begin{aligned}
\sum_{i=1}^{\rho}1\cdot|\eta_i|^2\sum_{i=1}^{\rho}1\cdot|\eta_i|^2+\sum_{i=1}^{\rho}1\cdot1^2\sum_{i=1}^{\rho}1\cdot1^2 &\geq 2\sum_{i=1}^{\rho}1\cdot|\eta_i|\cdot1\sum_{i=1}^{\rho}1\cdot|\eta_i|\cdot1,\\
2(\rho-1)M_1(\zeta)\cdot2(\rho-1)M_1(\zeta)+n\cdot n &\geq 2(E_{\mathcal{NS}o}(\zeta))^2,\\
4((\rho-1)M_1(\zeta))^2+n^2 &\geq 2(E_{\mathcal{NS}o}(\zeta))^2,\\
\sqrt{\frac{4((\rho-1)M_1(\zeta))^2+n^2}{2}} &\geq E_{\mathcal{NS}o}(\zeta),\\
E_{\mathcal{NS}o}(\zeta) &\leq \sqrt{2((\rho-1)M_1(\zeta))^2+\frac{n^2}{2}}.
\end{aligned}$$

This completes the proof. □

4. Applications on energy of a new variant Sombor matrix

Covid-19 is a disease caused by SARS-CoV-2 coronavirus, it is positive single stranded RNS virus containing protiens called as betacoronavirus. Fever, cough, sore throat, rhinorrhea, severe pneumonia and septic shock are the usual symptoms found in the patients affected by Covid-19. There is no exact antiviral drug yet in the treatment of Covid-19 disease, instead the existing drugs like Chloroquine, Hydroxychloroquine, Azithromycin, Remdesivir, Lopinavir, Ritonavir, Arbidol, Favipiravir, Theaflavin, Thalidomide, Ribavirin, etc., are used in the treatment of the patients affected by Covid-19. Every drug has a chemical structure which has certain interesting properties to study, the chemical graph is drawn from the chemical structure and topological indices are calculated, which is used in predicting physical properties of these drugs using QSPR/QSAR analysis. Energy of a graph is also a prominent component used in QSPR/QSAR analysis for predicting the physical properties. Our study focuses on 8 drugs namely Chloroquine, Hydroxychloroquine, Remdesivir, Lopinavir, Ritonavir, Arbidol, Theaflavin, and Thalidomide, which are potential drugs used in the treatment of COVID-19.

A data set containing physicochemical properties of drugs used in the treatment of COVID-19 is taken from . The Boiling point (BP), Enthalpy of vaporization (E), Flash point (FP), Molar refractivity (MR), Polar surface area (PSA), Polarizability (P), Surface tension (T), Molar volume (MV) along with

$E_{\mathcal{NS}o}(\zeta)$ is displayed in Table 2. The linear, quadratic and cubic regression analysis is conducted with these physicochemical properties using $E_{\mathcal{NS}o}(\zeta)$. In the following models n, F, SF and Sig represents the population, F-values, standard error of the estimate and statistically significant respectively.

The process of calculating the energy from its 3D chemical structure is illustrated in the flowchart.

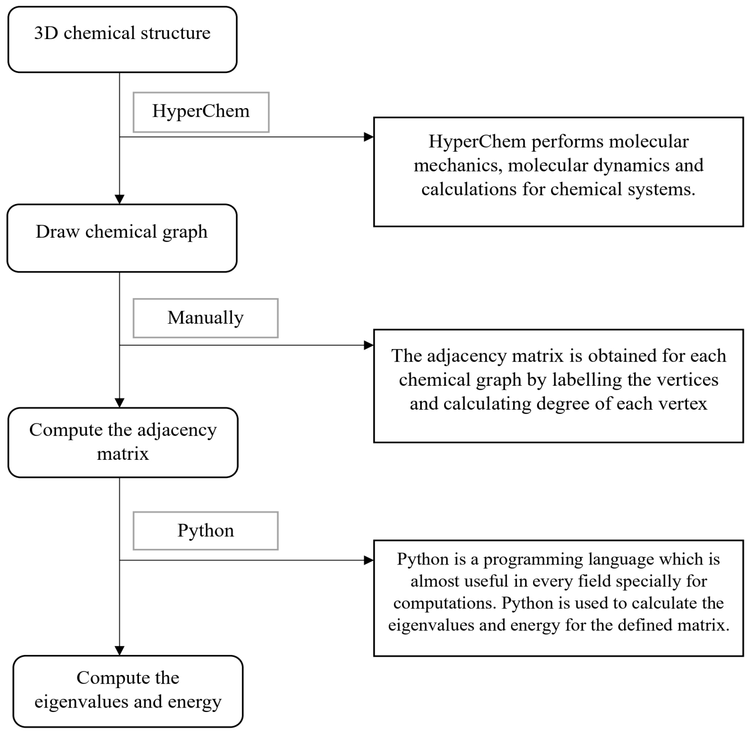

FIGURE 1. The figure depicts the process of calculating the energy from 3D chemical structure.

TABLE 1. Physicochemical properties of drugs used in the treatment of COVID-19 patients [14] and $E_{\mathcal{NS}o}(\zeta)$.

Name of Compounds	Formula	BP	E	FP	MR	PSA	P	T	MV	$E_{\mathcal{NS}o}(\zeta)$
Arbidol	$C_{22}H_{25}BrN_2O_3S$	591.8	91.5	311.7	121.9	80	48.3	45.3	347.3	179.5410
Chloroquine	$C_{18}H_{26}CIN_3$	460.6	72.1	232.3	97.4	28	38.6	44	287.9	130.0179
Hydroxychloroquine	$C_{18}H_{26}CIN_3O$	516.7	83	266.3	99	48	39.2	49.8	285.4	135.7314
Lopinavir	$C_{37}H_{48}N_4O_5$	924.2	140.8	512.7	179.2	120	71	49.5	540.5	284.0798
Remdesivir	$C_{27}H_{35}N_6O_8P$	–	–	–	149.5	213	59.3	62.3	409	264.5682
Ritonavir	$C_{37}H_{48}N_6O_5S_2$	947	144.4	526.6	198.9	202	78.9	53.7	581.7	308.0962
Thalidomide	$C_{13}H_{10}N_2O_4$	487.8	79.4	248.8	65.2	87	25.9	71.6	161	118.7019
Theaflavin	$C_{29}H_{24}O_{12}$	1003.9	153.5	336.5	137.3	218	54.4	138.6	301	266.7247

4.1. **Linear Regression Model. The linear regression model is given by**

$$PP = a(E_{\mathcal{NS}o}(\zeta)) + b$$

$$BP = 2.902(E_{\mathcal{NS}o}(\zeta)) + 114.676$$

$$n = 8 \ F = 78.186 \ SF = 64.970 \ Sig = 0.000$$

$$E = 0.421(E_{\mathcal{NS}o}(\zeta)) + 23.749$$

$$n = 8 \ F = 65.129 \ SF = 10.317 \ Sig = 0.000$$

$$FP = 1.392(E_{\mathcal{NS}o}(\zeta)) + 64.909$$

$$n = 8 \ F = 26.264 \ SF = 53.766 \ Sig = 0.004$$

$$MR = 0.540(E_{\mathcal{NS}o}(\zeta)) + 17.097$$

$$n = 8 \ F = 50.102 \ SF = 15.730 \ Sig = 0.000$$

$$P = 0.214(E_{\mathcal{NS}o}(\zeta)) + 6.763$$

$$n = 8 \ F = 50.260 \ SF = 6.228 \ Sig = 0.000$$

TABLE 2. The correlation coefficient value r for linear regression model between physicochemical properties and $E_{\mathcal{NS}o}(\zeta)$ of drugs used in the treatment of COVID-19 patients.

	BP	**E**	**FP**	**MR**	**PSA**	**P**	**T**	**MV**
$E_{\mathcal{NS}o}(\zeta)$	0.969	0.929	0.917	0.945	0.851	0.945	0.268	0.840

The linear regression models are depicted in the following figures.

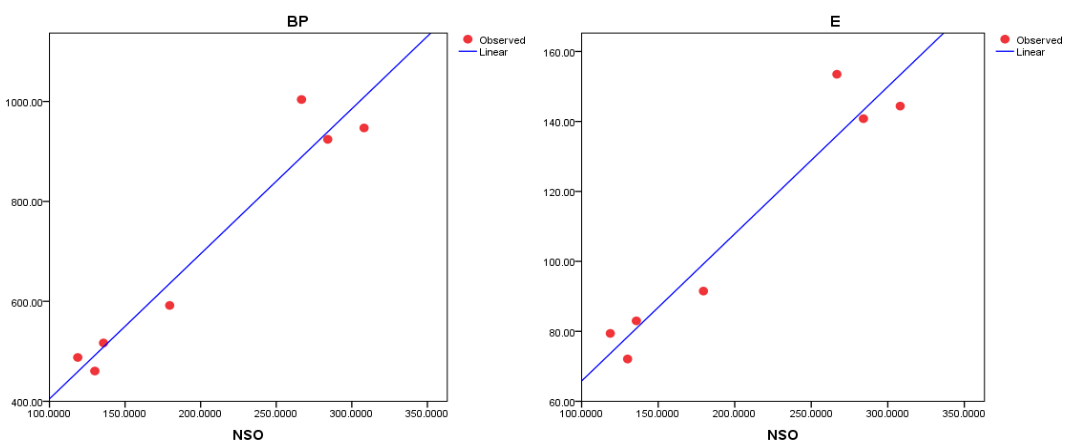

FIGURE 2. Linear regression model of BP and E with $E_{\mathcal{NS}o}(\zeta)$.

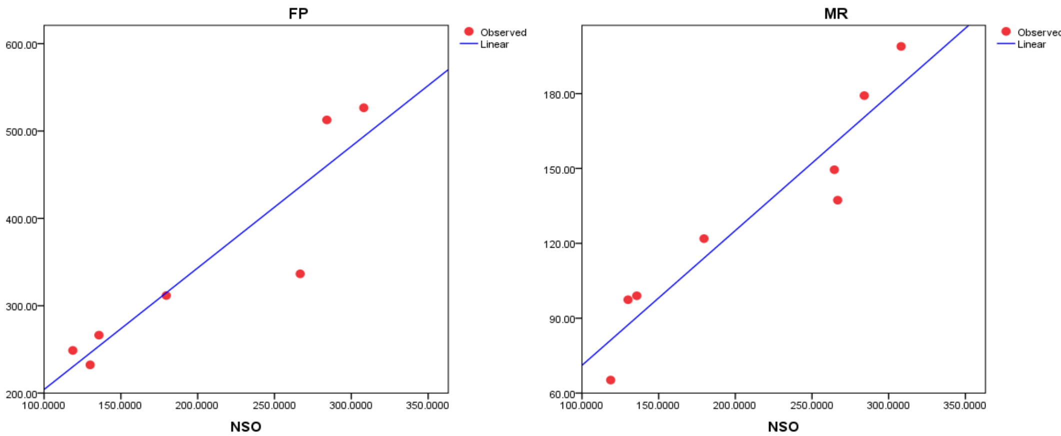

FIGURE 3. Linear regression model of FP and MR with $E_{\mathcal{NS}o}(\zeta)$.

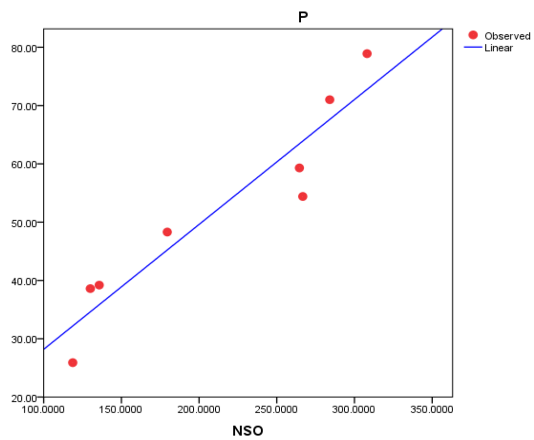

FIGURE 4. Linear regression model of P with $E_{\mathcal{NS}o}(\zeta)$.

4.2. **Quadratic Regression Model. The quadratic regression model is given by**

$$PP = a(E_{\mathcal{NS}o}(\zeta))^2 + b(E_{\mathcal{NS}o}(\zeta)) + c$$

$$BP = (-0.005)(E_{\mathcal{NS}o}(\zeta))^2 + 5.057(E_{\mathcal{NS}o}(\zeta)) + (-83.955)$$

$$n = 8 \;\; F = 33.539 \;\; SF = 70.286 \;\; Sig = 0.003$$

$$E = (-0.001)(E_{\mathcal{NS}o}(\zeta))^2 + 0.673(E_{\mathcal{NS}o}(\zeta)) + 0.518$$

$$n = 8 \;\; F = 65.129 \;\; SF = 10.317 \;\; Sig = 0.000$$

$$FP = 0.008(E_{\mathcal{NS}o}(\zeta))^2 + (-2.023)(E_{\mathcal{NS}o}(\zeta)) + 379.644$$

$$n = 8 \;\; F = 26.264 \;\; SF = 53.766 \;\; Sig = 0.004$$

$$MR = 0.001(E_{\mathcal{NS}o}(\zeta))^2 + 0.018(E_{\mathcal{NS}o}(\zeta)) + 65.158$$

$$n = 8 \;\; F = 22.389 \;\; SF = 16.699 \;\; Sig = 0.003$$

$$P = 0.001(E_{\mathcal{NS}o}(\zeta))^2 + 0.004(E_{\mathcal{NS}o}(\zeta)) + 26.109$$

$$n = 8 \;\; F = 22.513 \;\; SF = 6.604 \;\; Sig = 0.003$$

TABLE 3. The correlation coefficient value r for quadratic regression model between physicochemical properties and $E_{\mathcal{NS}o}(\zeta)$ of drugs used in the treatment of COVID-19 patients.

	BP	E	FP	MR	PSA	P	T	MV
$E_{\mathcal{NS}o}(\zeta)$	0.971	0.965	0.937	0.948	0.852	0.949	0.322	0.854

The quadratic regression models are depicted in the following figures.

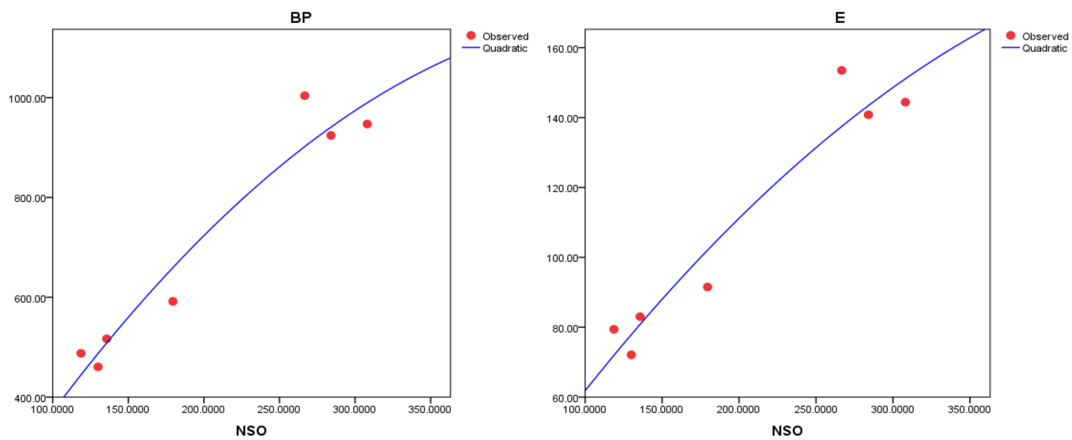

FIGURE 5. Quadratic regression model of BP and E with $E_{\mathcal{NS}o}(\zeta)$.

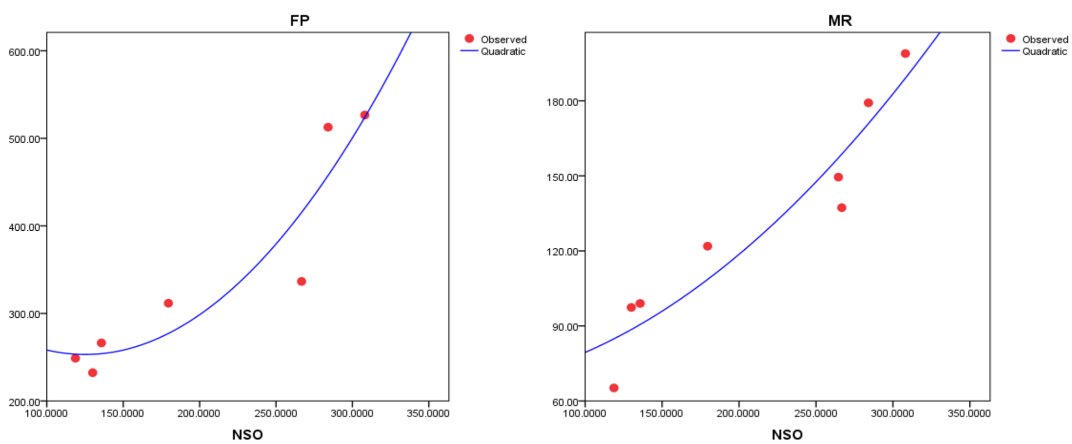

FIGURE 6. Quadratic regression model of FP and MR with $E_{\mathcal{NS}o}(\zeta)$.

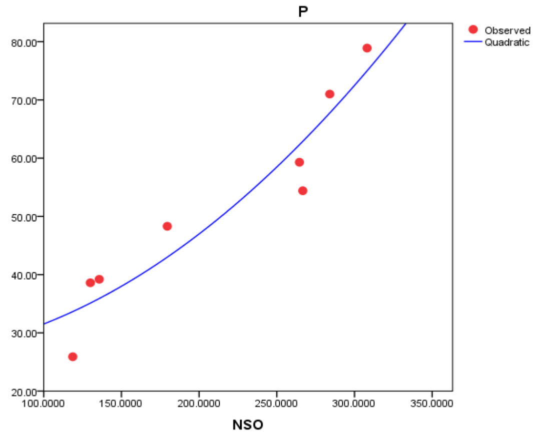

FIGURE 7. Quadratic regression model of P with $E_{\mathcal{NS}o}(\zeta)$.

4.3. **Cubic Regression Model. The cubic regression model is given by**

$$PP = a(E_{\mathcal{NS}o}(\zeta))^3 + b(E_{\mathcal{NS}o}(\zeta))^2 + c(E_{\mathcal{NS}o}(\zeta)) + d$$

$$BP = (-1.026 \times 10^{-5})(E_{\mathcal{NS}o}(\zeta))^3 + 23.661(E_{\mathcal{NS}o}(\zeta))^2 + 4.346(E_{\mathcal{NS}o}(\zeta)) + (-56.728)$$

$$n = 8 \ F = 35.203 \ SF = 68.696 \ Sig = 0.003$$

$$E = (-1.296 \times 10^{-6})(E_{\mathcal{NS}o}(\zeta))^3 + 25.815(E_{\mathcal{NS}o}(\zeta))^2 + 0.603(E_{\mathcal{NS}o}(\zeta)) + 2.115$$

$$n = 8 \ F = 28.057 \ SF = 11.143 \ Sig = 0.004$$

$$FP = 1.897 \times 10^{-5}(E_{\mathcal{NS}o}(\zeta))^3 + (-0.003)(E_{\mathcal{NS}o}(\zeta))^2 + 7.362(E_{\mathcal{NS}o}(\zeta)) + 264.319$$

$$n = 8 \ F = 15.244 \ SF = 51.191 \ Sig = 0.013$$

$$MR = 2.492 \times 10^{-6}(E_{\mathcal{NS}o}(\zeta))^3 + (-29.977)(E_{\mathcal{NS}o}(\zeta))^2 + 0.196(E_{\mathcal{NS}o}(\zeta)) + 57.999$$

$$n = 8 \ F = 23.533 \ SF = 16.328 \ Sig = 0.003$$

$$P = 9.991 \times 10^{-7}(E_{\mathcal{NS}o}(\zeta))^3 + (-29.922)(E_{\mathcal{NS}o}(\zeta))^2 + 0.076(E_{\mathcal{NS}o}(\zeta)) + 23.165$$

$$n = 8 \ F = 33.539 \ SF = 70.286 \ Sig = 0.003$$

TABLE 4. The correlation coefficient value r for quadratic regression model between physicochemical properties and $E_{\mathcal{NS}o}(\zeta)$ of drugs used in the treatment of COVID-19 patients.

	BP	**E**	**FP**	**MR**	**PSA**	**P**	**T**	**MV**
$E_{\mathcal{NS}o}(\zeta)$	0.973	0.966	0.940	0.951	0.853	0.951	0.351	0.863

The cubic regression models are depicted in the following figures.

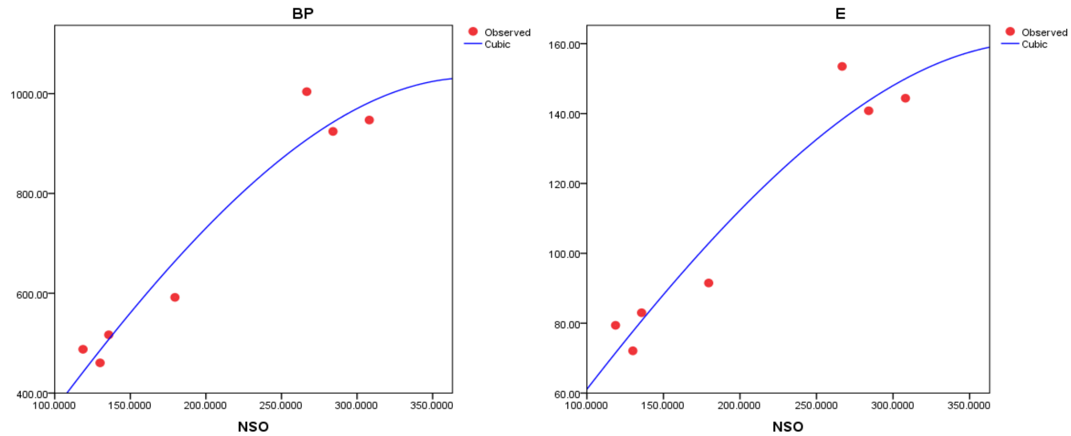

FIGURE 8. Cubic regression model of BP and E with $E_{\mathcal{NS}o}(\zeta)$.

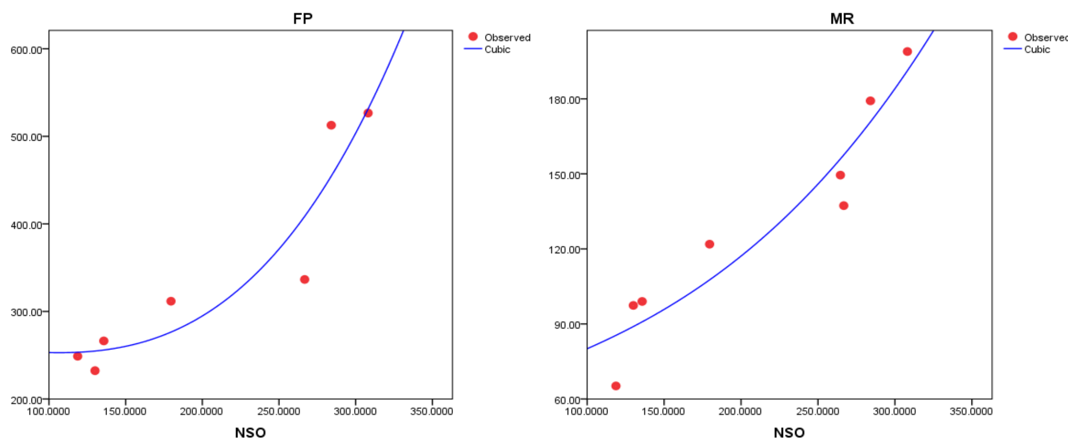

FIGURE 9. Cubic regression model of FP and MR with $E_{\mathcal{NS}o}(\zeta)$.

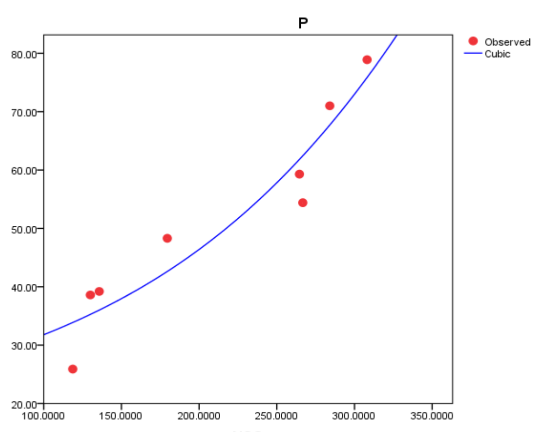

FIGURE 10. Cubic regression model of P with $E_{\mathcal{NS}o}(\zeta)$.

4.4. **Analysis.**

- The correlation coefficient r shows positive linear relationship between physicochemical properties and $E_{\mathcal{NS}o}(\zeta)$ with highest correlation for BP ($r = 0.969$) and lowest correlation for T ($r = 0.268$).
- The significant relationship for all properties with Sig < 0.05, indicates that it is statistical significance.
- The strongest fit are with BP, E, FP, MR and P with high F-values.
- The correlation coefficient r for quadratic model is improve compared to linear model with highest correlation for BP ($r = 0.971$) and lowest correlation for T ($r = 0.322$).
- Better fit for properties like BP, E, FP, MR and P, with significant F-values and Sig < 0.05.
- The correlation coefficient r for cubic model is high compared to linear and quadratic model with highest correlation for BP ($r = 0.973$) and lowest correlation for T ($r = 0.351$).
- Most accurate fit for properties like BP, E, FP, MR and P, with large F-values and Sig < 0.05.
- From all the three model, cubic model gives more improved correlation coefficient and $E_{\mathcal{NS}o}(\zeta)$ is able to predict the physicochemical properties of these drugs used in the treatment of COVID-19 patients.

5. Conclusion

In this paper, we introduce a novel variant of the Sombor matrix, denoted as $\mathcal{NS}o(\zeta)$, for a simple graph $\zeta(\mathcal{V}, \mathcal{E})$. The matrix is defined such that for $i \neq j$, the (i, j)-entry is given by $\sqrt{d_i^2 + d_j^2}$, where d_i represents the degree of the i^{th} vertex, and zero otherwise. The Sombor energy $E_{\mathcal{NS}o}(\zeta)$ is defined as the sum of the absolute values of these eigenvalues. We derive upper and lower bounds for both η_1 and $E_{\mathcal{NS}o}(\zeta)$ in terms of the first Zagreb index ($M_1(\zeta)$). As an application, we perform a Quantitative Structure-Property Relationship (QSPR) analysis using a dataset of drugs employed in the treatment of COVID-19 patients. We construct linear, quadratic, and cubic regression models to explore the relationship between the physicochemical properties of these drugs and their corresponding $E_{\mathcal{NS}o}(\zeta)$ values, with the models visualized through graphical representations.

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