ISSN: 1672 - 6553
JOURNAL OF DYNAMICS AND CONTROL
VOLUME 9 ISSUE 7: 60 - 77

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https://doi.org/10.71058/jodac.v9i7005

PYTHON-BASED COMPUTATION OF NSo(G) ENERGY: BOUNDS AND QSPR ANALYSIS ON COVID-19 DRUGS

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Abstract: *In this paper, we introduce a novel variant of the Sombor matrix, denoted by $\mathcal{NS}o(G)$, for a simple graph G. This matrix is defined such that for vertices $i \neq j$, 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 $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ denote the eigenvalues of $\mathcal{NS}o(G)$ with η_1 corresponding to the spectral radius, and let the associated Sombor energy $E_{\mathcal{NS}o}(G)$ be defined as the sum of the absolute values of these eigenvalues. We develop a Python-based computational framework to determine the spectrum and energy of $\mathcal{NS}o(G)$ and derive new upper and lower bounds for both η_1 and $E_{\mathcal{NS}o}(G)$ in terms of the first Zagreb index $M_1(G)$. As an application, we conduct a Quantitative Structure-Property Relationship (QSPR) analysis on a dataset comprising drugs used in the treatment of COVID-19, constructing linear regression models to explore the correlation between the physicochemical properties of these drugs and their corresponding $E_{\mathcal{NS}o}(G)$ values, with results illustrated through graphical representations.*

Keywords: *Sombor matrix, Sombor energy, spectral radius, COVID-19.*

1. Introduction

Let G be a simple graph, with vertex set $|V| = n$ and edge set $|E| = m$. The degree of a vertex $v \in V$ is the count of edges connected to v denoted by $d_G(v)$. The maximum(minimum) vertex and edge degree of a graph is denoted by $\Delta(\delta)$ and $\Delta'(\delta')$ respectively. A graph G is said to be complete if $\Delta = \delta = n - 1$ denoted by K_n. If a vertex set of a graph G is partitioned into two sets say $|M| = p$ and $|N| = q$ (partite sets) such that every edge meet both M and N then the graph is bipartite graph. If every vertex of M is adjacent to every vertex of N then the graph is complete bipartite graph denoted as $K_{p,q}$. The graph $K_{1,n-1}$ is called as star graph denoted by S_n and the graph $K_{p,p}$ is called equi-bipartite graph. The complement of a graph G denoted by $\overline{G}$ is a graph defined on same vertex set as of G such that if two vertices are adjacent in $\overline{G}$, then they are not adjacent in G. For more terminologies refer the following [12].

https://doi.org/10.71058/jodac.v9i7005

Topological indices are numerical descriptors derived from the structure of molecular graphs that capture essential features of chemical compounds. They are widely applied in QSAR/QSPR studies to predict physicochemical properties, biological activities, and to design new drugs. The first degree-based molecular descriptor, the Zagreb index, was developed by Gutman and Trinajstić [11]. It firstly emerged in the topological formula for conjugated molecules regarding their total π-electron energy. The first Zagreb index is defined as:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{e=uv \in E(G)} (d_G(u) + d_G(v)) \tag{1}$$

There is another topological index which is widely known and used in applications of graph theory specially in Chemistry. The Sombor index [9] is given by

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

Spectral graph theory has emerged as an active area of research in recent years, which explores the graph properties like eigenvalues and eigenvectors obtained from matrices such as the adjacency and Laplacian matrices. These eigenvalues, known collectively as the spectrum of the graph, capture rich structural and combinatorial information with significant applications in chemistry, physics, computer science, and network analysis. Among the important spectral parameters is the energy of a graph, introduced by Gutman in [10] which coincides with the π-electron energy of a conjugated hydrocarbon, as calculated with the Huckel molecular orbital (HMO) method.

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The adjacency matrix $A(G) = [a_{ij}]$ of order n is defined by

$$a_{ij} = \begin{cases} 1, & \text{if } v_i \text{isadjacent to } v_j, \\ 0, & \text{otherwise.} \end{cases}$$

If $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of $A(G)$, then the energy of the graph G, introduced by Gutman in [10], is given by

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

In 1994, Yang et al. [25] proposed the extended adjacency matrix $A_{ex}(G)$ for a graph G, and investigated the sum of the absolute values of its eigenvalues, which they termed the extended graph energy. Later, Ş. Burcu Bozkurt et al. [4] introduced the Randić matrix and studied the associated Randić energy, analyzing various structural properties of graphs.

In 2020, Lu Zheng et al. [15] defined the Arithmetic-Geometric matrix of graphs, establishing bounds for its spectral radius and energy. More recently, the Sombor matrix was introduced [8], derived from the Sombor index a degree-based topological index. Zhen Lin et al. [26] explored the spectral radius,

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energy, and Estrada index of the Sombor matrix, while Sumedha S. Shinde et al. [23] provided bounds on the Sombor eigenvalues and energy in terms of Hyper Zagreb and Zagreb indices. Recently Sakander Hayat et al. [21] defined edge-weighted matrix of a graph and obtained bounds in terms of first reformulated Zagreb index.

Several other graph matrices have been proposed in the literature, such as the degree sum matrix by H. S. Ramane et al. [19], degree square sum matrix [1], common neighbourhood matrix [24], eccentricity sum matrix [20], combined degree sum matrix [2], and the degree sum exponent distance matrix [22], all of which have attracted considerable research interest.

Motivated by these developments, we introduce a new variant of the Sombor matrix, denoted by $\mathcal{NS}o(G)$, defined as

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

where d_i represents the degree of the i^{th} vertex of G.

The characteristic polynomial of $\mathcal{NS}o(G)$ is given by $\psi(G,\eta) = \det(\eta I - \mathcal{NS}o(G)) = \eta^n + r_1\eta^{n-1} + \cdots + r_n$, where I is the identity matrix of order n. Since $\mathcal{NS}o(G)$ is a real symmetric matrix, all its eigenvalues are real. Arranged in non-increasing order, the eigenvalues are $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$, with respective multiplicities $\tau_1, \tau_2, \dots, \tau_n$. Thus, the spectrum of $\mathcal{NS}o(G)$ can be represented as

$$Spectra(\mathcal{NS}o(G)) = \begin{pmatrix} \eta_1 & \eta_2 & \cdots & \eta_n \\ \tau_1 & \tau_2 & \cdots & \tau_n \end{pmatrix},$$

where η_1 is the spectral radius.

Finally, the Sombor energy associated with $\mathcal{NS}o(G)$ is defined by

$$E_{\mathcal{NS}o}(G) = \sum_{i=1}^{n} |\eta_i|.$$

2. Computational Implementation

2.1 Python program

In this section, we utilize Python, a powerful high-level programming language well-suited for numerical computations and data analysis, to implement our proposed methodology. Python's rich ecosystem of scientific libraries, such as NumPy, makes it particularly effective for handling matrix operations and eigenvalue computations, which are essential for spectral graph theory.

https://doi.org/10.71058/jodac.v9i7005

Below, we present the Python program developed for our research, which takes as input the degree sequence of a simple graph G and constructs the new variant Sombor matrix $\mathcal{NS}o(G)$. The program then computes its eigenvalues and calculates the corresponding Sombor energy $E_{\mathcal{NS}o}(G)$, providing a computational tool that supports the theoretical results established in this paper. Moreover, this program can be readily modified to compute the spectrum and energy of other degree-based matrices, such as the degree sum matrix, degree square sum matrix, and combined degree sum matrix.

```
#Python program to compute Sombor energy NSo(G).

import numpy as np

# Input the degree sequence
degrees = list(map(int, input("Enter degree sequence separated by spaces: ").split()))
n = len(degrees)

# Construct the matrix NSo(G)
A = np.zeros((n, n))
for i in range(n):
    for j in range(n):
        if i != j:
            A[i, j] = np.sqrt(degrees[i]**2 + degrees[j]**2)

# Compute eigenvalues and energy
eigenvalues = np.linalg.eigvals(A)
energy = np.sum(np.abs(eigenvalues))

# Output
print("\nMatrix NSo(G):")
print(np.array2string(A, formatter={'float_kind':lambda x: "%.2f" % x}))
print("\nEigenvalues:", eigenvalues)
print("\nSombor Energy:", energy)
```

Figure 1. Python program.

Example: Let G be a simple graph as shown in the Figure 1.2.

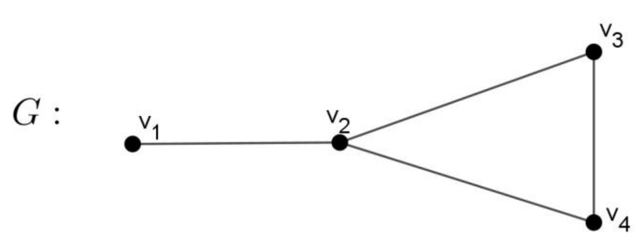

Figure 2. Simple graph G.

The degree of each vertex of G is $d_1 = 1$, $d_2 = 3$, $d_3 = 2$, $d_4 = 2$. A new variant of Sombor matrix $\mathcal{NS}o(G)$ of G is

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$$\mathcal{NS}o(G)=\begin{bmatrix}0 & \sqrt{10} & \sqrt{5} & \sqrt{5}\\ \sqrt{10} & 0 & \sqrt{13} & \sqrt{13}\\ \sqrt{5} & \sqrt{13} & 0 & 2\sqrt{2}\\ \sqrt{5} & \sqrt{13} & 2\sqrt{2} & 0\end{bmatrix}$$

The eigenvalues are $\eta_1 = 8.9153$, $\eta_2 = -4.04155$, $\eta_3 = -2.82843$, $\eta_4 = -2.04532$.

The Sombor energy $E_{\mathcal{NS}o}(G)$ is 17.8306.

Remark 2.1 *The Sombor matrix $SOM(G)$ and energy is defined in [8], we try to relate the newly variant Sombor matrix $\mathcal{NS}o(G)$ with $SOM(G)$. The matrix and eigenvalues of the matrix are equal if and only if $G = K_n$ or $G = \overline{K_n}$. Further the energy of $\mathcal{NS}o(G) = 2\eta_1$ (η_1 being the spectral radius) for any graph G, which is not the same in the case of energy of $SOM(G)$.*

3. Preliminaries

Lemma 3.1 *[5] (Cauchy Schwartz inequality) Let a_i and b_i, $1 \le i \le s$ be any real numbers, then*

$$\left(\sum_{i=1}^{s} a_i b_i\right)^2 \le \left(\sum_{i=1}^{s} a_i^2\right)\left(\sum_{i=1}^{s} b_i^2\right) \tag{3}$$

Lemma 3.2 *[13] Let a_i, $1 \le i \le s$ be any real numbers, then*

$$\left(\sum_{i=1}^{s} |a_i|\right)^2 \ge \left(\sum_{i=1}^{s} |a_i|^2\right) \tag{4}$$

Lemma 3.3 *[16] (Ozeki inequality) If a_i and b_i, $(1 \le i \le s)$ are non-negative real numbers then*

$$\sum_{i=1}^{s} a_i^2 \sum_{i=1}^{s} b_i^2 - \left[\sum_{i=1}^{s} a_i b_i\right]^2 \le \frac{n^2}{4}(N_1N_2 - n_1n_2)^2 \tag{5}$$

where $N_1 = max_{1\le i\le s}\{a_i\}$, $N_2 = max_{1\le i\le s}\{b_i\}$, $n_1 = min_{1\le i\le s}\{a_i\}$, $n_2 = min_{1\le i\le s}\{b_i\}$.

Lemma 3.4 *[18] Suppose a_i and b_i, $1 \le i \le s$ are positive real numbers, then*

$$\sum_{i=1}^{s} a_i^2 \sum_{i=1}^{s} b_i^2 \le \frac{1}{4}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right)^2 \left(\sum_{i=1}^{s} a_i b_i\right)^2 \tag{6}$$

where $N_1 = max_{1\le i\le s}\{a_i\}$, $N_2 = max_{1\le i\le s}\{b_i\}$, $n_1 = min_{1\le i\le s}\{a_i\}$, $n_2 = min_{1\le i\le s}\{b_i\}$.

Lemma 3.5 *[3] Suppose a_i and b_i, $1 \le i \le s$ are positive real numbers, then*

$$\left|s\sum_{i=1}^{s} a_i b_i - \sum_{i=1}^{s} a_i \sum_{i=1}^{s} b_i\right| \le \alpha(s)(A-a)(B-b) \tag{7}$$

where a, b, A and B are real constants, that for each i, $1 \le i \le s$, $a \le a_i \le A$ and $b \le b_i \le B$. Further, $\alpha(s) = s\lfloor\frac{s}{2}\rfloor\left(1 - \frac{1}{s}\lfloor\frac{s}{2}\rfloor\right)$.

Lemma 3.6 *[6] Let a_i and b_i, $1 \le i \le s$ are nonnegative real numbers, then*

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$$\sum_{i=1}^{s} b_i^2 + tT\sum_{i=1}^{s} a_i^2 \leq (t+T)(\sum_{i=1}^{s} a_i b_i) \quad (8)$$

where t and T are real constants, so that for each i, $1 \leq i \leq s$, holds, $ta_i \leq b_i \leq Ta_i$.

Lemma 3.7 *[14] Let $a_1 \geq a_2 \geq \cdots \geq a_s \geq 0$ be a sequence of non-negative real numbers. Then*

$$\sum_{i=1}^{s} a_i + s(s-1)(\prod_{i=1}^{s} a_i)^{1/s} \leq \left[\sum_{i=1}^{s} \sqrt{a_i}\right]^2 \leq (s-1)\sum_{i=1}^{s} a_i + s(\prod_{i=1}^{s} a_i)^{1/s} \quad (9)$$

Lemma 3.8 *[7] Let a_i, b_i, c_i and d_i are sequences of real numbers and p_i, q_i are non-negative for $i = 1,2,\ldots,s$. Then the following inequality is valid*

$$\sum_{i=1}^{s} p_i a_i^2 \sum_{i=1}^{s} q_i b_i^2 + \sum_{i=1}^{s} p_i c_i^2 \sum_{i=1}^{s} q_i d_i^2 \geq 2\sum_{i=1}^{s} p_i a_i c_i \sum_{i=1}^{s} q_i b_i d_i \quad (10)$$

4. Main Results

Lemma 4.1 *Consider a simple connected graph G with d_i representing the degree of the i^{th} vertex. Let $\mathcal{NS}o(G)$ be a new variant Sombor matrix of the graph G with eigenvalues $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ then,*

$$\sum_{i=1}^{n} \eta_i = 0$$

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

Proof: Since

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

Where, $\sum_{i<j}(d_i^2 + d_j^2) = (n-1)M_1(G)$

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

Theorem 4.2 *Let G be a connected graph with n vertices and η_1 be the spectral radius (the largest eigenvalue), then*

https://doi.org/10.71058/jodac.v9i7005

$$\eta_1 \leq \sqrt{\frac{2(n-1)^2 M_1(G)}{n}} \tag{11}$$

with equality holds if and only if G is a regular graph.

Proof: Since $\sum_{i=1}^{n} \eta_i = 0$ it can be rewritten as $\sum_{i=2}^{n} \eta_i = -\eta_1$. Further $(\sum_{i=1}^{n} (\eta_i)^2) = 2(n-1)M_1(G)$, $(\sum_{i=2}^{n} (\eta_i)^2) = (\sum_{i=1}^{n} (\eta_i)^2 - (\eta_1)^2) = (2(n-1)M_1(G) - (\eta_1)^2)$ and $(\sum_{i=2}^{n} 1) = (n-1)$.

Substituting $a_i = 1$ and $b_i = \eta_i$ in Lemma 3.1, we get

$$(-\eta_1)^2 \leq (n-1)(2(n-1)M_1(G) - (\eta_1)^2)$$

$$(-\eta_1)^2 \leq 2(n-1)^2 M_1(G) - (n-1)(\eta_1)^2$$

$$(-\eta_1)^2 \leq 2(n-1)^2 M_1(G) - n(\eta_1)^2 + (\eta_1)^2$$

$$n(\eta_1)^2 \leq 2(n-1)^2 M_1(G)$$

$$\eta_1 \leq \sqrt{\frac{2(n-1)^2 M_1(G)}{n}}$$

One can verify that the equality holds if and only if G is a regular graph.

Theorem 4.3 *Let G be a connected graph with n vertices then*

$$\sqrt{2(n-1)M_1(G)} \leq E_{\mathcal{NS}o(G)} \leq \sqrt{2n(n-1)M_1(G)} \tag{12}$$

Proof: Since $E_{\mathcal{NS}o(G)} = \sum_{i=1}^{n} |\eta_i|$, $\sum_{i=1}^{n} 1 = n$ and $\sum_{i=1}^{n} |\eta_i|^2 = 2(n-1)M_1(G)$

Substituting $a_i = |\eta_i|$ and $b_i = 1$ in Lemma 3.1, we get

$$E_{\mathcal{NS}o(G)}^2 \leq 2n(n-1)M_1(G)$$

$$E_{\mathcal{NS}o(G)} \leq \sqrt{2n(n-1)M_1(G)}$$

Also, substituting $a_i = |\eta_i|$ in Lemma 3.2, we get

$$E_{\mathcal{NS}o(G)}^2 \geq 2(n-1)M_1(G)$$

$$E_{\mathcal{NS}o(G)} \geq \sqrt{2(n-1)M_1(G)}$$

This gives us both the upper and lower bound.

Theorem 4.4 *Let G be a connected graph with n vertices then*

$$E_{\mathcal{NS}o(G)} \geq \frac{2\sqrt{2(n-1)M_1(G)|\eta_1||\eta_n|}}{|\eta_1|+|\eta_n|} \tag{13}$$

https://doi.org/10.71058/jodac.v9i7005

Proof: Let $|\eta_1|$ and $|\eta_n|$ be the largest and the smallest eigenvalues. Since $E_{\mathcal{NSo}(G)} = \sum_{i=1}^{n} |\eta_i|$ and $\sum_{i=1}^{n} |\eta_i|^2 = 2(n-1)M_1(G)$

Substituting $a_i = |\eta_i|$, $b_i = 1$, $N_1 = |\eta_1|$, $n_1 = |\eta_n|$, $N_2 = 1$ and $n_2 = 1$ in Lemma 3.4, we get

$$\sum_{i=1}^{n} |\eta_i|^2 \sum_{i=1}^{n} 1 \leq \frac{1}{4}\left(\sqrt{\frac{|\eta_1|}{|\eta_n|}} + \sqrt{\frac{|\eta_n|}{|\eta_1|}}\right)^2 \left(\sum_{i=1}^{n} |\eta_i|\right)^2$$

$$2(n-1)M_1(G)n \leq \frac{1}{4}\left(\frac{(|\eta_1|+|\eta_n|)}{\sqrt{|\eta_n||\eta_1|}}\right)^2 E_{\mathcal{NSo}(G)}^2$$

$$2n(n-1)M_1(G) \leq \frac{1}{4}\left(\frac{(|\eta_1|+|\eta_n|)^2}{|\eta_n||\eta_1|}\right) E_{\mathcal{NSo}(G)}^2$$

$$\frac{8n(n-1)M_1(G)|\eta_n||\eta_1|}{(|\eta_1|+|\eta_n|)^2} \leq E_{\mathcal{NSo}(G)}^2$$

$$E_{\mathcal{NSo}(G)} \geq \sqrt{\frac{8n(n-1)M_1(G)|\eta_1||\eta_n|}{(|\eta_1|+|\eta_n|)^2}}$$

$$E_{\mathcal{NSo}(G)} \geq \frac{2\sqrt{2n(n-1)M_1(G)|\eta_1||\eta_n|}}{|\eta_1|+|\eta_n|}$$

Theorem 4.5 *Let G be a connected graph with n vertices then*

$$E_{\mathcal{NSo}(G)} \geq \frac{\sqrt{8n(n-1)M_1(G)-n^2(|\eta_1|-|\eta_n|)^2}}{2} \tag{14}$$

Proof: Let $|\eta_1|$ and $|\eta_n|$ be the largest and the smallest eigenvalues. Since $E_{\mathcal{NSo}(G)} = \sum_{i=1}^{n} |\eta_i|$ and $\sum_{i=1}^{n} |\eta_i|^2 = 2(n-1)M_1(G)$

Substituting $a_i = |\eta_i|$, $b_i = 1$, $N_1 = |\eta_1|$, $n_1 = |\eta_n|$, $N_2 = 1$ and $n_2 = 1$ in Lemma 3.3, we get

$$\sum_{i=1}^{n} |\eta_i|^2 \sum_{i=1}^{n} 1 - \left(\sum_{i=1}^{n} |\eta_i|\right)^2 \leq \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2$$

$$2(n-1)M_1(G)n - E_{\mathcal{NSo}(G)}^2 \leq \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2$$

$$2n(n-1)M_1(G) - \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2 \leq E_{\mathcal{NSo}(G)}^2$$

$$\frac{8n(n-1)M_1(G)-n^2(|\eta_1|-|\eta_n|)^2}{4} \leq E_{\mathcal{NSo}(G)}^2$$

https://doi.org/10.71058/jodac.v9i7005

$$E_{\mathcal{NS}o(G)} \geq \frac{\sqrt{8n(n-1)M_1(G) - n^2(|\eta_1| - |\eta_n|)^2}}{2}$$

Theorem 4.6 *Let G be a connected graph with n vertices then*

$$E_{\mathcal{NS}o(G)} \leq |\eta_1| + \sqrt{(2(n-1)M_1(G) - |\eta_1|^2)(n-1)} \quad (15)$$

Proof: Let $|\eta_1|$ be the largest eigenvalue. Since $E_{\mathcal{NS}o(G)} = \sum_{i=1}^{n} |\eta_i|$,

$$E_{\mathcal{NS}o(G)} - |\eta_1| = \sum_{i=2}^{n} |\eta_i|$$

Squaring both sides and applying Lemma 3.1, we get

$$(E_{\mathcal{NS}o(G)} - |\eta_1|)^2 = \left(\sum_{i=2}^{n} |\eta_i|\right)^2$$

$$(E_{\mathcal{NS}o(G)} - |\eta_1|)^2 = \left(\sum_{i=2}^{n} |\eta_i| \cdot 1\right)^2 \leq \left(\sum_{i=2}^{n} |\eta_i|^2\right)\left(\sum_{i=2}^{n} 1^2\right)$$

$$(E_{\mathcal{NS}o(G)} - |\eta_1|)^2 \leq (2(n-1)M_1(G) - |\eta_1|^2)(n-1)$$

$$(E_{\mathcal{NS}o(G)} - |\eta_1|) \leq \sqrt{(2(n-1)M_1(G) - |\eta_1|^2)(n-1)}$$

$$E_{\mathcal{NS}o(G)} \leq |\eta_1| + \sqrt{(2(n-1)M_1(G) - |\eta_1|^2)(n-1)}$$

Theorem 4.7 *Let G be a connected graph with n vertices then*

$$\sqrt{2(n-1)M_1(G) + n(n-1)[det(\mathcal{NS}o(G))]^{2/n}} \leq \left(E_{\mathcal{NS}o(G)}\right)$$

$$\leq \sqrt{2(n-1)^2 M_1(G) + n[det(\mathcal{NS}o(G))]^{2/n}}$$

Proof: Since $E_{\mathcal{NS}o(G)} = \sum_{i=1}^{n} |\eta_i|$,

Substituting $a_i = \eta_i^2$ in Lemma 3.7, we get

$$\sum_{i=1}^{n} \eta_i^2 + n(n-1)\left(\prod_{i=1}^{n} \eta_i^2\right)^{1/n} \leq \left(\sum_{i=2}^{n} \sqrt{\eta_i^2}\right)^2 \leq (n-1)\sum_{i=1}^{n} \eta_i^2 + n\left(\prod_{i=1}^{n} \eta_i^2\right)^{1/n}$$

$$2(n-1)M_1(G) + n(n-1)[det(\mathcal{NS}o(G))]^{2/n} \leq \left(E_{\mathcal{NS}o(G)}\right)^2$$

$$\leq (n-1)2(n-1)M_1(G) + n[det(\mathcal{NS}o(G))]^{2/n}$$

$$2(n-1)M_1(G) + n(n-1)[det(\mathcal{NS}o(G))]^{2/n} \leq \left(E_{\mathcal{NS}o(G)}\right)^2$$

https://doi.org/10.71058/jodac.v9i7005

$$\leq 2(n-1)^2 M_1(G) + n[det(\mathcal{NS}o(G))]^{2/n}$$

$$\sqrt{2(n-1)M_1(G) + n(n-1)[det(\mathcal{NS}o(G))]^{2/n}} \leq \left(E_{\mathcal{NS}o(G)}\right)$$

$$\leq \sqrt{2(n-1)^2 M_1(G) + n[det(\mathcal{NS}o(G))]^{2/n}}$$

Theorem 4.8 *Let G be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(G)$. Then*

$$E_{\mathcal{NS}o}(G) \geq \sqrt{2n(n-1)M_1(G) - \alpha(n)(|\eta_1| - |\eta_n|)^2} \tag{16}$$

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 $\mathcal{NS}o(G)$. By putting $a_i = |\eta_i| = b_i$, $A = |\eta_1| = B$ and $a = |\eta_n| = b$ in Lemma 3.5, we get

$$|n\sum_{i=1}^{n} |\eta_i|^2 - (\sum_{i=1}^{n} |\eta_i|)^2| \leq \alpha(n)(|\eta_1| - |\eta_n|)^2$$

$$|2n(n-1)M_1(G) - (E_{\mathcal{NS}o}(G))^2| \leq \alpha(n)(|\eta_1| - |\eta_n|)^2$$

$$2n(n-1)M_1(G) - \alpha(n)(|\eta_1| - |\eta_n|)^2 \leq (E_{\mathcal{NS}o}(G))^2$$

$$E_{\mathcal{NS}o}(G) \geq \sqrt{2n(n-1)M_1(G) - \alpha(n)(|\eta_1| - |\eta_n|)^2}$$

Theorem 4.9 *Let G be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(G)$. Then*

$$E_{\mathcal{NS}o}(G) \geq \frac{n + 2(n-1)M_1(G)(\eta_n\eta_1)}{\eta_n + \eta_1} \tag{17}$$

with equality holds if and only if G is a complete graph K_2.

Proof: Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(G)$. By putting $a_i = |\eta_i|$, $b_i = 1$, $t = \eta_n$ and $T = \eta_1$, in Lemma 3.6, we get

$$\sum_{i=1}^{n} 1^2 + \eta_n\eta_1 \sum_{i=1}^{n} |\eta_i|^2 \leq (\eta_n + \eta_1)(\sum_{i=1}^{n} |\eta_i|)$$

$$n + 2(n-1)M_1(G)(\eta_n\eta_1) \leq (\eta_n + \eta_1)E_{\mathcal{NS}o}(G)$$

$$E_{\mathcal{NS}o}(G) \geq \frac{n + 2(n-1)M_1(G)(\eta_n\eta_1)}{\eta_n + \eta_1}$$

Theorem 4.10 *Let G be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(G)$. Then*

$$E_{\mathcal{NS}o}(G) \geq \frac{2(n-1)M_1(G)+n(\eta_1\eta_n)}{\eta_1+\eta_n} \tag{18}$$

Proof: Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(G)$. By putting $a_i = 1$, $b_i = |\eta_i|$, $t = \eta_n$ and $T = \eta_1$, in Lemma 3.6, we get

$$\sum_{i=1}^{n} |\eta_i|^2 + \eta_n\eta_1 \sum_{i=1}^{n} 1^2 \leq (\eta_n + \eta_1)(\sum_{i=1}^{n} |\eta_i|)$$

$$2(n-1)M_1(G) + n(\eta_n\eta_1) \leq (\eta_n + \eta_1)E_{\mathcal{NS}o}(G)$$

$$E_{\mathcal{NS}o}(G) \geq \frac{2(n-1)M_1(G)+n(\eta_1\eta_n)}{\eta_1+\eta_n}$$

Theorem 4.11 *Let G be a non-empty graph with n vertices. Then*

$$E_{\mathcal{NS}o}(G) \leq \sqrt{2((n-1)M_1(G))^2 + \frac{n^2}{2}} \tag{19}$$

Proof: Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{NS}o(G)$. Substituting $a_i = |\eta_i| = b_i$ and $c_i = d_i = p_i = q_i = 1$ in Lemma 3.8, we get

$$\sum_{i=1}^{n} 1 \cdot |\eta_i|^2 \sum_{i=1}^{n} 1 \cdot |\eta_i|^2 + \sum_{i=1}^{n} 1 \cdot 1^2 \sum_{i=1}^{n} 1 \cdot 1^2 \geq 2\sum_{i=1}^{n} 1 \cdot |\eta_i| \cdot 1 \sum_{i=1}^{n} 1 \cdot |\eta_i| \cdot 1$$

$$2(n-1)M_1(G) \cdot 2(n-1)M_1(G) + n \cdot n \geq 2(E_{\mathcal{NS}o}(G))^2$$

$$4((n-1)M_1(G))^2 + n^2 \geq 2(E_{\mathcal{NS}o}(G))^2$$

$$\sqrt{\frac{4((n-1)M_1(G))^2+n^2}{2}} \geq E_{\mathcal{NS}o}(G)$$

$$E_{\mathcal{NS}o}(G) \leq \sqrt{2((n-1)M_1(G))^2 + \frac{n^2}{2}}$$

5. 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

https://doi.org/10.71058/jodac.v9i7005

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 $E_{\mathcal{NS}o}(G)$ is displayed in Table 2. The linear, quadratic and cubic regression analysis is conducted with these physicochemical properties using $E_{\mathcal{NS}o}(G)$. 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 following flowchart.

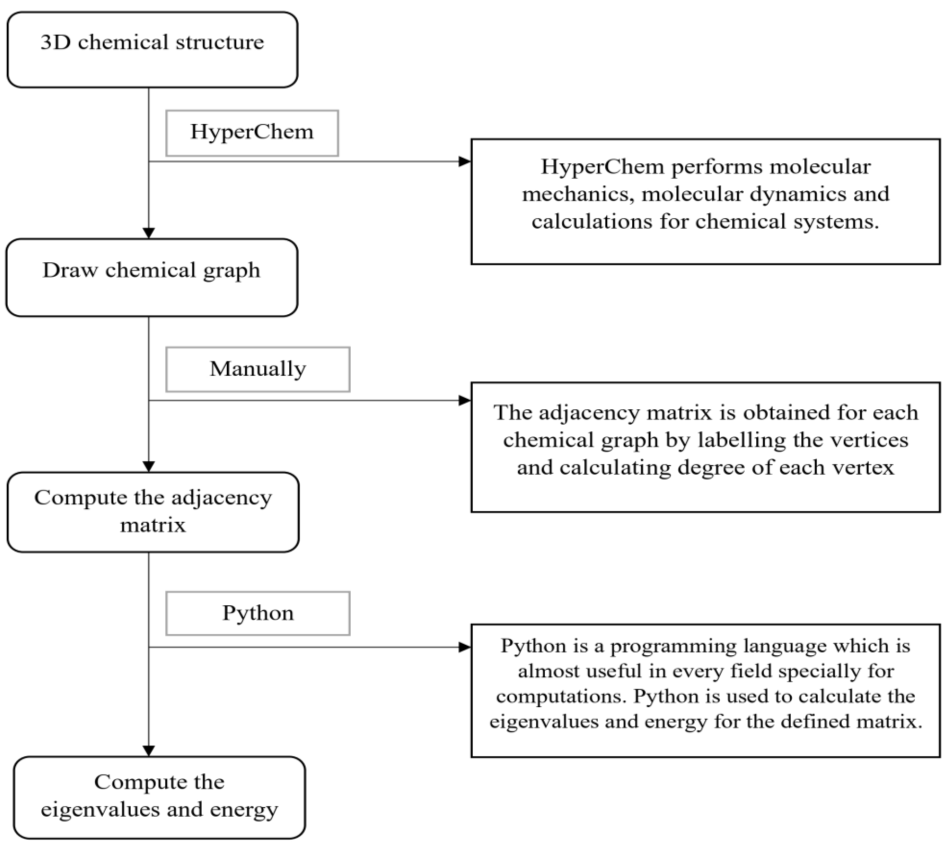

Figure 3. The figure depicts the process of calculating the energy from 3D chemical structure.

https://doi.org/10.71058/jodac.v9i7005

Table 1. Physicochemical properties of drugs used in the treatment of COVID-19 patients [17] and $E_{\mathcal{NSo}}(G)$.

Name of compounds	Formula	BP	E	FP	MR	PSA	P	T	MV	$E_{\mathcal{NSo}}(G)$
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

5.1 Linear Regression Model

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

	BP	E	FP	MR	PSA	P	T	MV
$E_{\mathcal{NSo}}(G)$	0.969	0.929	0.917	0.945	0.851	0.945	0.268	0.840

The linear regression model is given by

$$PP = a(E_{\mathcal{NSo}}(G)) + b$$

$$BP = 2.902(E_{\mathcal{NSo}}(G)) + 114.676$$

https://doi.org/10.71058/jodac.v9i7005

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

$$E = 0.421(E_{\mathcal{NSo}}(G)) + 23.749$$

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

$$FP = 1.392(E_{\mathcal{NSo}}(G)) + 64.909$$

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

$$MR = 0.540(E_{\mathcal{NSo}}(G)) + 17.097$$

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

$$P = 0.214(E_{\mathcal{NSo}}(G)) + 6.763$$

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

The linear regression models are depicted in the following figures.

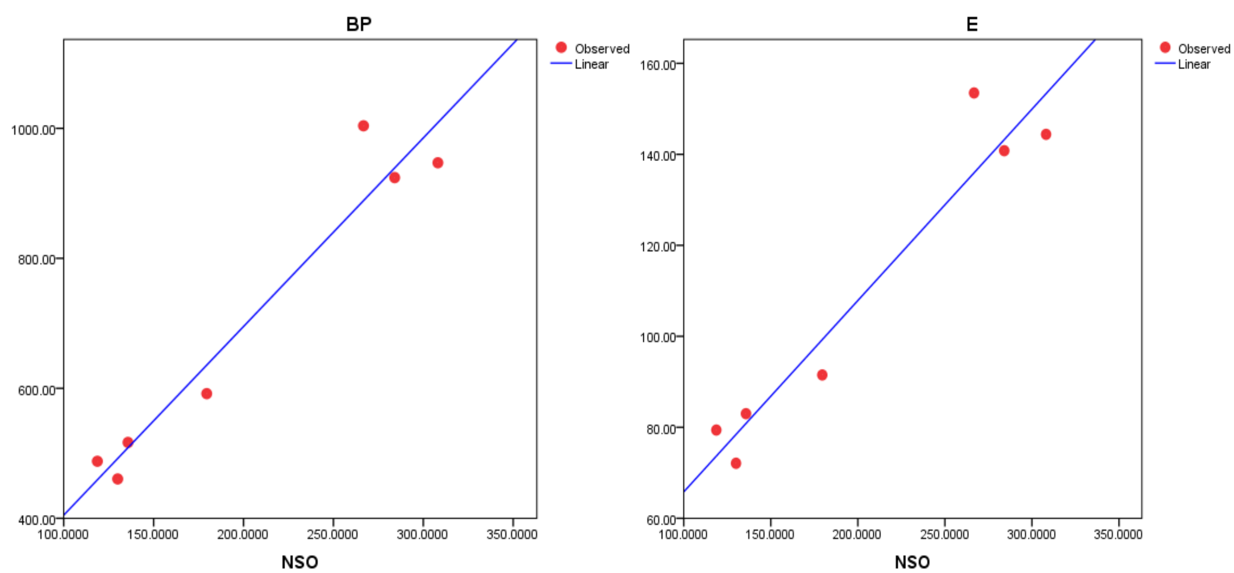

Figure 4. Linear regression model of BP and E with $E_{\mathcal{NSo}}(G)$

https://doi.org/10.71058/jodac.v9i7005

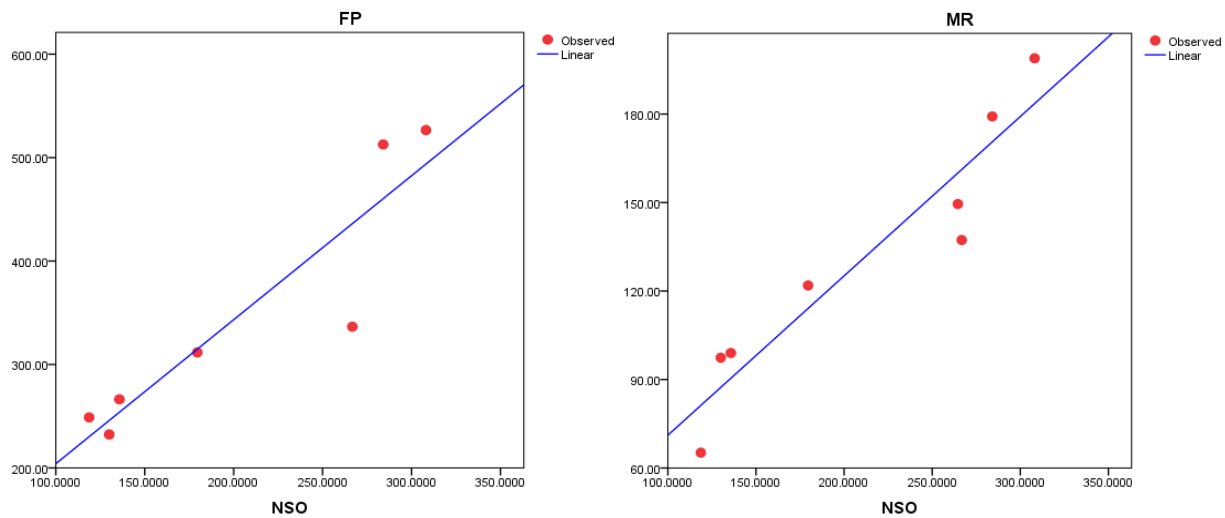

Figure 5. Linear regression model of FP and MR with $E_{\mathcal{N}\mathcal{S}o}(G)$

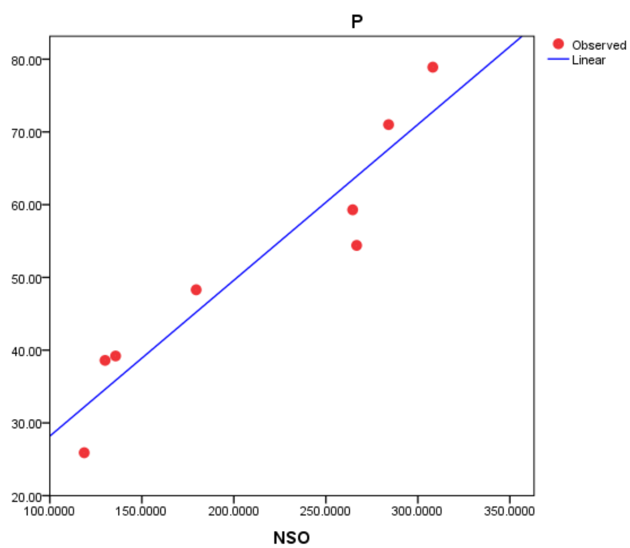

Figure 6. Linear regression model of P with $E_{\mathcal{N}\mathcal{S}o}(G)$

5.2 Analysis

The following analysis can be made from the linear regression model:

- The correlation coefficients r indicate a positive linear relationship between the Sombor energy $E_{\mathcal{N}\mathcal{S}o}(G)$ and the physicochemical properties of the drugs. The highest correlation is observed with BP ($r = 0.969$), followed by MR ($r = 0.945$), P ($r = 0.945$), E ($r = 0.929$), FP ($r = 0.917$), PSA ($r = 0.851$), and MV ($r = 0.840$). The lowest correlation is with T ($r = 0.268$), indicating

https://doi.org/10.71058/jodac.v9i7005

a weak relationship.

- All linear regression models show statistical significance with $Sig < 0.05$, demonstrating that $E_{\mathcal{N}\mathcal{S}o}(G)$ is a meaningful predictor for these physicochemical properties.
- The F-values are notably high for BP, E, MR, and P, reflecting strong model fits and suggesting that variations in these physicochemical properties are well explained by $E_{\mathcal{N}\mathcal{S}o}(G)$.
- Thus, $E_{\mathcal{N}\mathcal{S}o}(G)$ can effectively predict several key physicochemical properties of drugs used in the treatment of COVID-19 patients, especially BP, MR, P, E, and FP. However, due to the low correlation with T, $E_{\mathcal{N}\mathcal{S}o}(G)$ does not serve as a reliable predictor for this property.

6. Conclusion

In this paper, we introduce a novel variant of the Sombor matrix, denoted as $\mathcal{N}\mathcal{S}o(G)$, for a simple graph G. 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 $E_{\mathcal{N}\mathcal{S}o}(G)$ is defined as the sum of the absolute values of these eigenvalues. We derive upper and lower bounds for both η_1 and $E_{\mathcal{N}\mathcal{S}o}(G)$ in terms of the first Zagreb index $(M_1(G))$. 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 regression models to explore the relationship between the physicochemical properties of these drugs and their corresponding $E_{\mathcal{N}\mathcal{S}o}(G)$ values, with the models visualized through graphical representations.

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