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Original Article

Study on Weighted Sombor Indices and Its QSPR Analysis on Medical Drugs

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Abstract *- Chemical Graph Theory has emerged as a vital tool in accelerating drug discovery by reducing costs and time frames while addressing critical challenges in bioavailability and toxicity during the early stages of development. This study introduces novel topological indices, namely Weighted Sombor indices and Reduced Weighted Sombor indices, derived from the M-Polynomial of the graph$G$. These indices are evaluated for specific classes of graphs using their M-Polynomials. Additionally, Quantitative Structure-Property Relationship (QSPR) studies have been done on antiviral drugs utilized in COVID-19 medication, including Chloroquine, Hydroxychloroquine, Remdesivir, Lopinavir, Ritonavir, Arbidol, and Theaflavin. The predictive potential of the indices Reduced Sombor SO_r, Weighted Sombor SO_w, Reduced Weighted Sombor SO_{rw} They are evaluated concerning physicochemical properties such as Boiling Point* (BP), *Surface Tension* (T)*, Molar Volume* (MV)*, and Polar Surface Area* (PSA)*. These findings underscore the applicability of the proposed indices in Chemical Graph Theory and their relevance in computational drug discovery.*

Keywords *- Degree-based topological index, Weighted Sombor index, Reduced Weighted Sombor index, M-polynomial, Covid-19, QSPR studies.*

1. Introduction

In a molecular graph G, the set of vertices V of G encodes atoms, and the edges E of G encodes the bonding between atoms in a molecule. Let G be a chemical graph containing $V(G)$ vertices and $E(G)$ edges. The degree of a vertex v in $V(G)$, denoted by d_v, is the total number of edges associated with v. Topological indices are mathematical descriptors of molecular graphs that predict chemical compounds' physiochemical, biological, toxicological and structural properties [14]. The topological indices emerged when the eminent Chemist Wiener found the first topological index, the Wiener Index [7,8].
Many topological indices were introduced, including degree- and distance-based topological indices [9-12]. Among the degree-based topological indices, Randic index, Zagreb index, ABC index and Sombor index play a vital role in QSPR analysis in chemical graph theory. Among the distance-based indices, Wiener and Hosoya indexes are widely used in both QSAR and QSPR analyses [3,5,6,7,8,20].

To study the strong relationship between the chemical characteristics and molecular structure of chemical compounds, topological indices were defined, and they helped researchers better understand the physical features, chemical reactivity, and biological activity, avoiding expensive laboratory experiments. [24-26,29-31]. In recent years, advancements in technology have significantly accelerated the development of chemical and pharmaceutical techniques, leading to the emergence of numerous novel nanomaterials, crystalline substances, and drugs annually. Evaluating the chemical properties of these newly developed compounds and pharmaceuticals demands extensive experimentation, substantially increasing the workload for researchers in the chemical and pharmaceutical fields. However, chemical experiments have revealed a robust relationship between the molecular structure's topology and its physical, chemical, and biological properties.

In this paper, motivated by various applications of Sombor and Zagreb indices, a new topological index and its reduced form are introduced, viz, Weighted Sombor Index and Reduced Weighted Sombor Index. M-polynomials are mathematical tools used in graph and chemical graph theory to encode information about a graph's structure. They are particularly useful in applications like chemistry for analyzing molecular graphs [1,23]. Using M-polynomials, topological indices can be derived

directly through mathematical manipulations, avoiding the need to calculate indices individually. Here, the new indices are derived from the graph's M-Polynomial. Weighted Sombor indices of some special class of graphs are computed from their M-Polynomials. Also, Quantitative Structure-Property Relationships (QSPR) studies have been done on the chemical drugs used for COVID-19 treatment, such as Chloroquine, Hydroxychloroquine, Remdesivir, Lopinavir, Ritonavir, Arbidol and Theaflavin. Here, a better predictive nature of the topological indices SO_w, SO_r, SO_{rw} The physico-chemical properties such as Boiling Point (BP), Surface Tension (T), Molar Volume (MV), and Polar Surface Area (PSA) are obtained, which contributes to the advanced applications in Chemical graph theory.

2. Basic Results

The Zagreb index, invented at the initial stage, investigated how the total π electron energy depends on the chemical structure of molecules. [9,10] Till now, a large number of topological indices have been defined and studied in detail.

The First Zagreb indices $M_1(G)$ is defined as $M_1(G) = \sum_{uv\in E(G)} d_u + d_v$.

The Second Zagreb indices $M_2(G)$ is defined as $M_2(G) = \sum_{uv\in E(G)} d_u * d_v$.

The Randic indices $R(G)$ is defined as $R(G) = \sum_{uv\in E(G)} \frac{1}{d_u d_v}$.

The Forgotten indices are defined as $F(G) = \sum_{uv\in E(G)} {d_u}^2 + {d_v}^2$.

The Sombor indices are defined as $\mathrm{SO}(G) = \sum_{uv\in E(G)} \sqrt{{d_u}^2 + {d_v}^2}$.

Inspired by the definition and applications of the Sombor index, researchers have introduced its modified forms [11]. They are the Modified Sombor index. ${}^{m}\mathrm{SO}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{{d_u}^2+{d_v}^2}}$,

Multiplicative Sombor index $\mathrm{SO}II(G) = \prod_{uv\in E(G)} \sqrt{{d_u}^2 + {d_v}^2}$,

Reduced Sombor index $\mathrm{SO}_r(G) = \sum_{uv\in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}$,

Reverse Sombor index $\mathrm{RSO}(G) = \sum_{uv\in E(G)} \sqrt{(\Delta - d_u + 1)^2 + (\Delta - d_v + 1)^2}$,

δ-Sombor index ${}^{\delta}\mathrm{SO}(G) = \sum_{uv\in E(G)} (d_u - \delta - 1)^2 + (d_v - \delta - 1)^2$, etc.

Usually, topological indices are calculated by using their standard mathematical formulas. Instead of calculating them separately, several algebraic polynomials have been developed, which generate the topological indices by different operations like differentiation, integration, or a mix of both.

For example, the distance-based topological indices Wiener and Hyper Wiener indexes can be derived from Hosoya Polynomial [29]. The Neighborhood degree sum topological indices can be derived from NM Polynomials [22].

In 2015, Detsch and Klavzar introduced M-Polynomial to determine the degree-based topological indices [1]. So far, for different chemical structures, numerous degree based topological indices are calculated with the help of their M-polynomials.

Definition 2.1:[1] The M polynomial of a graph G defined as $M(G;x,y) = \sum_{\delta\le i\le j\le \Delta} \varnothing_{i,j}(G) x^i y^j$, where $\delta = \min\{d_u : u\epsilon V(G)\}$, $\Delta = \max\{d_u : u\epsilon V(G)$ and $\varnothing_{i,j}(G)$ is the number of edges $uv\epsilon E(G)$ such that $d_u = i \; and \; d_v = j$; $i,j \ge 1$.

A degree-based topological index of a graph G can be represented as $I(G) = \sum_{uv\in E(G)} f(d_u, d_v)$, where $f(d_u, d_v)$ is the function of d_u, d_v Which depends on the mathematical definition of the index.

Here, we list some operators that will be utilized in the context of the manuscript. They are

$$D_x f(x,y) = x\frac{\partial f(x,y)}{\partial x}, D_y f(x,y) = y\frac{\partial f(x,y)}{\partial y}$$

$$S_x f(x,y) = \int_0^x \frac{f(t,y)}{t}\,dt\,, S_y f(x,y) = \int_0^y \frac{f(x,t)}{t}\,\mathrm{d}t$$

$$D_x^{\frac{1}{2}}\big(f(x,y)\big) = \sqrt{x\frac{\partial f(x,y)}{\partial x}}\sqrt{f(x,y)}$$

$$D_y^{\frac{1}{2}}\big(f(x,y)\big) = \sqrt{y\frac{\partial f(x,y)}{\partial y}}\sqrt{f(x,y)}$$

$$S_x^{\frac{1}{2}}(f(x,y)) = \sqrt{\int_0^x \frac{f(t,y)}{t}\,dt}\sqrt{f(x,y)}$$

$$S_y^{\frac{1}{2}}(f(x,y)) = \sqrt{\int_0^y \frac{f(x,t)}{t}\,dt}\sqrt{f(x,y)}$$

$$J\big(f(x,y)\big) = f(x,x)$$

$$Q_\propto f(x,y) = x^\propto f(x,y)$$

$$P_x\left(h\big(x^\alpha, y^\beta\big)\right) = h(x^{\alpha^2}, y^\beta)$$

$$P_y\left(h\big(x^\alpha, y^\beta\big)\right) = h(x^\alpha, y^{\beta^2}).$$

3. Main Results

3.1. Definitions and Derivations

The new topological indices were introduced: Weighted Sombor and Reduced Weighted Sombor indices. Also, they were derived from the M-Polynomial of the graph G.

First, we present the definitions of Weighted Sombor indices. $SO_w(G)$, Reduced Weighted Sombor indices $SO_{rw}(G)$.

Definition 3.1: For a graph G, the Weighted Sombor indices are defined as

$$\mathrm{SO}_w(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2}\sqrt{{d_u}^2 + {d_v}^2}.$$

For a graph G, the Reduced Weighted Sombor indices is defined as $\mathrm{SO}_{rw}(G) = \sum_{uv\in E(G)} \frac{(d_u-1)+(d_v-1)}{2}\sqrt{(d_u-1)^2+(d_v-1)^2}$.

Definition 3.2: The edge partition of the graph G be defined in two ways as $M(i,j)(G) = |\{uv \in E(G): d_u = i, d_v = j\}|$

Definition 3.3: Let G be a graph. We introduce the M-polynomial of $M(G,x,y) = \sum M(i,j)x^i y^j$

Next, we propose a derivation formula for these indices: Sombor indices $SO(G)$, Weighted Sombor indices. $SO_w(G)$, Reduced Weighted Sombor indices $SO_{rw}(G)$ of a graph G, with the help of the M-Polynomial of the graph.

Theorem 3.1: Let G be a graph, and the Sombor index is $SO(G) = \sum_{uv\in E(G)} f(d_u, d_v)$, where $f(x,y) = \sqrt{x^2+y^2}$. Then

$SO(G) = D_x^{\frac{1}{2}} J P_y P_x M(G;x,y)/_{x=1}$, where $M(G;x,y)$ is the M-Polynomial of G.

Proof:

$$\frac{1}{2}D_x^{\frac{1}{2}}JP_yP_xM(G;x,y) = D_x^{\frac{1}{2}}JP_yP_x\sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)x^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)\ D_x^{\frac{1}{2}}JP_yP_xx^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)\,D_x^{\frac{1}{2}}J\left(x^{i^2}y^{j^2}\right)$$
$$= \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)\ D_x^{\frac{1}{2}}\left(x^{i^2+j^2}\right)$$
$$= \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)\sqrt{i^2+j^2}\left(x^{i^2+j^2}\right)$$

Therefore

$$D_x^{\frac{1}{2}}JP_yP_xM(G;x,y)/_{x=1} = \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)\sqrt{i^2+j^2}$$
$$= \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)f(i,j)$$

So $SO(G) = \sum_{uv\in E(G)}f(d_u,d_v) = \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)f(i,j)$.

Theorem 3.2: Let G be a graph, and the Weighted Sombor index is $SO_w(G) = \sum_{uv\in E(G)}f(d_u,d_v)$, where $f(x,y) = \frac{x+y}{2}\sqrt{x^2+y^2}$. Then $SO_w(G) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x\left(D_x+D_y\right)M(G;x,y)/_{x=1}$, where $M(G;x,y)$ Is the M-Polynomial of G.

Proof:

$$\frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x\left(D_x+D_y\right)M(G;x,y) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x\left(D_x+D_y\right)\sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)x^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)\frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x\left(D_x+D_y\right)x^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta}\frac{i+j}{2}\varnothing_{i,j}(G)\frac{1}{2}D_x^{\frac{1}{2}}JP_yP_xx^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta}\frac{i+j}{2}\varnothing_{i,j}(G)\frac{1}{2}D_x^{\frac{1}{2}}J\left(x^{i^2}y^{j^2}\right)$$
$$= \sum_{\delta\le i\le j\le\Delta}\frac{i+j}{2}\varnothing_{i,j}(G)\frac{1}{2}D_x^{\frac{1}{2}}\left(x^{i^2+j^2}\right)$$
$$= \sum_{\delta\le i\le j\le\Delta}\frac{i+j}{2}\varnothing_{i,j}(G)\sqrt{i^2+j^2}\left(x^{i^2+j^2}\right)$$

Therefore $\frac{1}{2}D_x^{\frac{1}{2}}Q_{-1}JP_yP_x\left(D_x+D_y\right)M(G;x,y)/_{x=1} = \sum_{\delta\le i\le j\le\Delta}\varnothing_{i,j}(G)$

$$\frac{i+j}{2}\sqrt{i^2+j^2} = \sum_{\delta\le i\le j\le\delta}\varnothing_{i,j}(G)f(i,j)$$

So $SO_{rw}(G) = \sum_{uv\in E(G)} f\,(d_u, d_v) = \sum_{\delta\le i\le j\le\delta} \varnothing_{i,j}\,(G) f(i,j)$

Theorem 3.3: Let G be a graph, and the Reduced Weighted Sombor index is $SO_{rw}(G) = \sum_{uv\in E(G)}\ f(d_u, d_v)$, where $f(x,y) = \frac{x+y-2}{2}\sqrt{(x-1)^2+(y-1)^2}$.

Then $O_{rw}(G) = \frac{1}{2} D_x^{\frac{1}{2}} Q_{-1} J P_y P_x \left(Q_{-1}D_x + Q_{-1}D_y\right) M(G;x,y)/_{x=1}$, where $M(G;x,y)$ Is the M-Polynomial of G.

Proof:

$$\frac{1}{2} D_x^{\frac{1}{2}} Q_{-1} J P_y P_x \left(Q_{-1}D_x + Q_{-1}D_y\right) M(G;x,y) = \frac{1}{2} D_x^{\frac{1}{2}} Q_{-1} J P_y P_x \left(Q_{-1}D_x + Q_{-1}D_y\right)$$

$$\sum_{\delta\le i\le j\le\Delta} \varnothing_{i,j}\,(G) x^i y^j = \sum_{\delta\le i\le j\le\Delta} \varnothing_{i,j}\,(G) \frac{1}{2} D_x^{\frac{1}{2}} Q_{-1} J P_y P_x \left(Q_{-1}D_x + Q_{-1}D_y\right) x^i y^j$$

$$= \sum_{\delta\le i\le j\le\Delta} \frac{i+j-2}{2} \varnothing_{i,j}(G) \frac{1}{2} D_x^{\frac{1}{2}} J P_y P_x x^{i-1} y^{j-1}$$

$$= \sum_{\delta\le i\le j\le\Delta} \frac{i+j-2}{2} \varnothing_{i,j}(G) \frac{1}{2} D_x^{\frac{1}{2}} J \left(x^{(i-1)^2} y^{(j-1)^2}\right)$$

$$= \sum_{\delta\le i\le j\le\Delta} \frac{i+j-2}{2} \varnothing_{i,j}(G) \frac{1}{2} D_x^{\frac{1}{2}} \left(x^{(i-1)^2+(j-1)^2}\right)$$

$$= \sum_{\delta\le i\le j\le\Delta} \frac{i+j-2}{2} \varnothing_{i,j}(G) \sqrt{(i-1)^2+(j-1)^2} \left(x^{(i-1)^2+(j-1)^2}\right).$$

Therefore

$$\frac{1}{2} D_x^{\frac{1}{2}} Q_{-1} J P_y P_x \left(Q_{-1}D_x + Q_{-1}D_y\right) M(G;x,y)/_{x=1}$$

$$= \sum_{\delta\le i\le j\le\Delta} \frac{i+j-2}{2} \varnothing_{i,j}(G) \sqrt{(i-1)^2+(j-1)^2}$$

$$= \sum_{\delta\le i\le j\le\Delta} \varnothing_{i,j}\,(G) f(i,j)$$

So $SO_{rw}(G) = \sum_{uv\in E(G)} f\,(d_u, d_v) = \sum_{\delta\le i\le j\le\Delta} \varnothing_{i,j}\,(G) f(i,j)$

3.2. Weighted Sombor Index of some Class of Graphs

Weighted Sombor index of Path graph, Complete graph, Cycle graph, Star graph, Complete Bipartite graph, Wheel graph, Ladder graph and Friendship graph were derived from their corresponding M-Polynomials.

Theorem 3.4

(i) The $SO_w(G)$of path graph P_n is $3\sqrt{5} + (n-3)4\sqrt{2}$

(ii) The $SO_w(G)$ of the complete graph K_n is $\sqrt{2}n(n-1)^3$

(iii) The $SO_w(G)$of the cycle C_n is $4\sqrt{2}n$

(iv) The $SO_w(G)$of the star graph $K_{1,n}$ is $\frac{n(n+1)}{2}\sqrt{n^2+1}$

(v) The $SO_w(G)$of the complete bipartite graph $K_{m,n}$ is $\frac{mn(m+n)}{2}\sqrt{m^2+n^2}$

(vi) The $SO_w(G)$of the wheel graph W_n is $9\sqrt{2}(n-1) + \frac{(n-1)(n+2)}{2}\sqrt{(n-1)^2+9}$

(vii) The $SO_w(G)$of the ladder graph L_n is $27\sqrt{2}n + 10\sqrt{13} - 64\sqrt{2}$

(viii) The $SO_w(G)$of the friendship graph F_n is $4\sqrt{2}n + 4n(n+1)\sqrt{n^2+1}$

Proof

In path graph P_n, there are two vertices of degree 1, and all other n-2 vertices are of degree 2.

For P_n, the M-Polynomial is $2xy^2 + (n-3)x^2y^2, n \geq 3$.

$SO_w(P_n) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)(2xy^2 + (n-3)x^2y^2) = 3\sqrt{5} + (n-3)4\sqrt{2}$

In K_n, there are n vertices of degree $n-1$ and $n(n-1)/2$ edges with end vertex degree $(n-1, n-1)$.
For K_n, the M-Polynomial is $\frac{n(n-1)}{2}x^{n-1}y^{n-1}$

$$SO_w(K_n) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)(\frac{n(n-1)}{2}x^{n-1}y^{n-1}) = \frac{n(n+1)}{2}\sqrt{n^2+1}$$

In C_n, there are n edges of the end vertex degree (2,2)

For C_n, the M-Polynomial is $nx^2y^2, n \geq 3$

$$SO_w(C_n) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)(nx^2y^2, n \geq 3) = 4\sqrt{2}n$$

In $K_{1,n}$, there are n edges with end vertex degree $(1, n)$

For $K_{1,n}$, the M-Polynomial is nxy^n

$$SO_w(K_{1,n}) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)(nxy^n) = \frac{n(n+1)}{2}\sqrt{n^2+1}.$$

In $K_{m,n}$, there are mn edges with end vertex degree (n, m). For $K_{m,n}$, the M-Polynomial is mnx^my^n

$$SO_w(K_{m,n}) = \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)(mnx^my^n) = \frac{mn(m+n)}{2}\sqrt{m^2+n^2}$$

In W_n, there are $n-1$ edges with end vertex degree (3,3) and $n-1$ edges with end vertex degree $(n-1,3)$. For W_n, the M-Polynomial is $(n-1)x^3y^3 + (n-1)x^3y^{n-1}$

$$\begin{aligned} SO_w(W_n) &= \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)((n-1)x^3y^3 + (n-1)x^3y^{n-1}) \\ &= 9\sqrt{2}(n-1) + \frac{(n-1)(n+2)}{2}\sqrt{(n-1)^2+9} \end{aligned}$$

In L_n, there are 2 edges of the end vertex degree (2,2), 4 edges of the end vertex degree (2,3) and 3n-8 edges of the end vertex degree (3,3)
For L_n, the M-Polynomial is $2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3$

$$\begin{aligned} SO_w(L_n) &= \frac{1}{2}D_x^{\frac{1}{2}}JP_yP_x(D_x + D_y)(2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3) \\ &= 27\sqrt{2}n + 10\sqrt{13} - 64\sqrt{2} \end{aligned}$$

In F_n, there are n edges of the end vertex degree (2,2) and 2n edges of the end vertex degree $(2n, 2)$
For F_n, the M-Polynomial is $nx^2y^2 + 2nx^2y^{2n}$

$$SO_w(F_n) = \frac{1}{2} D_x^{\frac{1}{2}} J P_y P_x \left(D_x + D_y\right)\left(nx^2y^2 + 2nx^2y^{2n}\right)$$
$$= 4\sqrt{2}n + 4n(n+1)\sqrt{n^2+1}.$$

3.3. Analysis of Antiviral Drugs

In this subsection, we compute the Weighted Sombor Indices of chemical compounds used in the treatment of Covid 19. Also, the M-polynomial of these structures is shown with 3D graphical representations.

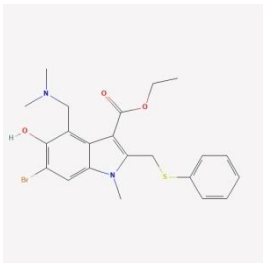
The antiviral medications used to treat COVID-19, including chloroquine, hydroxychloroquine, remdesivir, lopinavir, ritonavir, arbidol, theaflavin, and thalidomide, are examined [25, 28]. As stated in [33], "Since World War II, hydroxychloroquine, which is produced from 4-aminoquinoline, has been used as an antimalarial medication and to treat rheumatoid arthritis, lupus erythematosus, skin disorders, and other inflammatory ailments. Likewise, another antimalarial medication that works well for autoimmune disorders is chloroquine, which inhibits RNA transcription and DNA replication by interfering with nuclear proteins. Remdesivir is a nucleotide analogue that suppresses viral RNA replication and shows potential against a variety of viruses. It was first created as an experimental antiviral to treat Ebola. The HIV protease inhibitor lopinavir, which is frequently used in conjunction with ritonavir, prolongs its half-life by inhibiting cytochrome P450. Abidol is a non-nucleoside antiviral with wide antiviral action that works against influenza A and B viruses. However, there is little evidence to support their use for cancer, heart disease, or cholesterol. Theaflavins—natural polymers made from oxidized catechins in plant leaves—are used for digestive problems, dental health, and other conditions. Thalidomide, known for causing congenital defects like phocomelia, is now employed in treating autoimmune disorders such as psoriasis, systemic lupus erythematosus, and inflammatory gastrointestinal diseases".

"Figure 1 shows the molecular structures of Chloroquine, Hydroxychloroquine, Remdesivir, Lopinavir, Ritonavir, Arbidol, Theaflavin, and Thalidomide drugs."

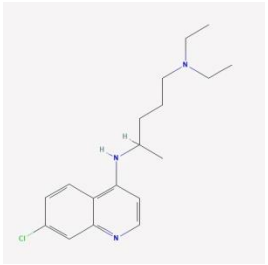
"Table 1 shows the edge–degree partition of the drugs. Also, Table 2 shows the M-Polynomial and its 3D Plot using Wolfram Alpha."

Table 1. Edge-Degree Partition of Drugs

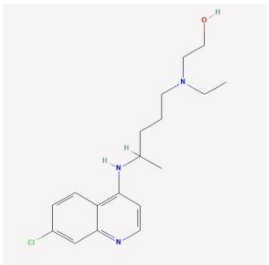
Drugs / (d_x, d_y)	**(1,2)**	**(1,3)**	**(1,4)**	**(2,2)**	**(2,3)**	**(2,4)**	**(3,3)**	**(3,4)**
Chloroquine (C)	2	2		5	12		2	
Hydroxychloroquine (HC)	2	2		6	12		2	
Remdesivir (Re)	2	5	2	9	14	4	6	2
Lopinavir (L)		8		14	20		7	
Ritonavir (Ri)		8		14	20		7	
Arbidol (A)	1	6		6	9		9	
Theaflavin (Th)		10			22		14	



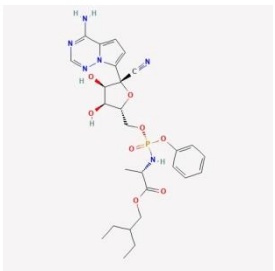
Arbidol (A)



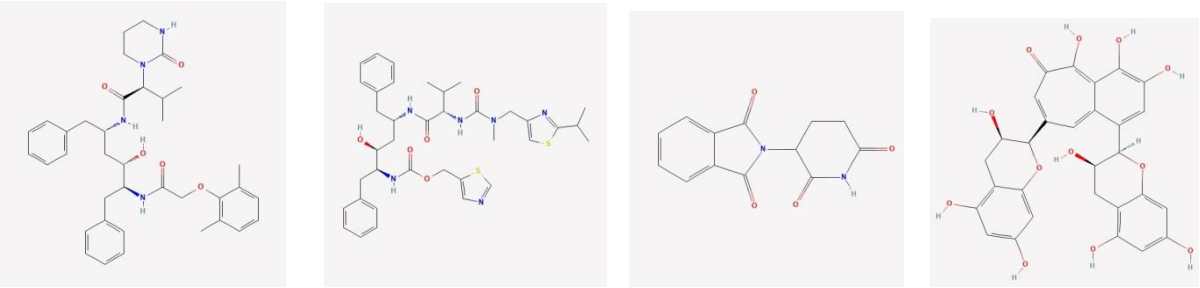
Chloroquine (C)



Hydroxychloroquine (HC)



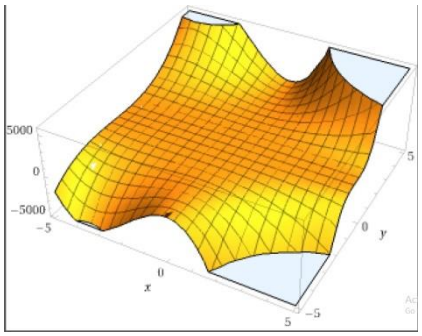
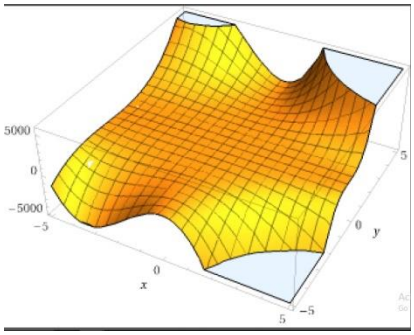
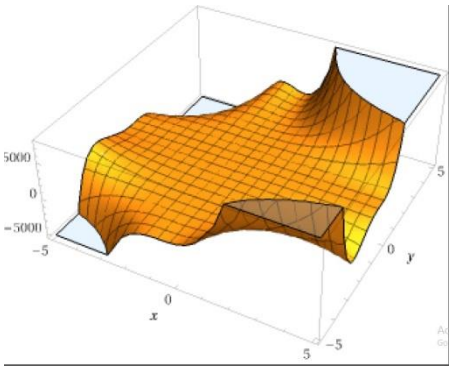
Remdesivir (Re)



Lopinavir (L) Ritonavir (Ri) Thalidomide (T) Theaflavin (Th)

Fig. 1 Chemical Structure of Antiviral drugs used in Covid-19 Treatment.

Table 2. M-Polynomial and its 3D Plot of each Drug

Drugs	M-Polynomial	3-D Plot
Chloroquine (C)	$M(G, x, y) = 2xy^2 + 2xy^3 + 5x^2y^2 + 12x^2y^3 + 2x^3y^3.$	
Hydroxychloroquine (HC)	$M(G, x, y) = 2xy^2 + 2xy^3 + 6x^2y^2 + 12x^2y^3 + 2x^3y^3.$	
Remdesivir (Re)	$M(G, x, y) = 2xy^2 + 5xy^3 + 2xy^4 + 9x^2y^2 + 14x^2y^3 + 4x^2y^4 + 6x^3y^3 + 2x^3y^4.$	

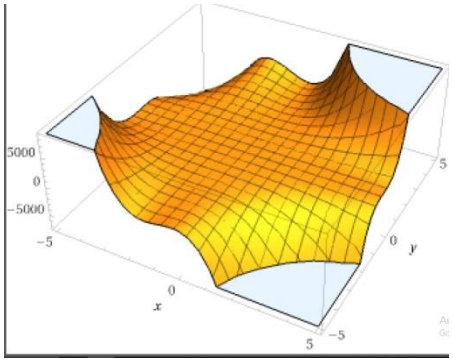
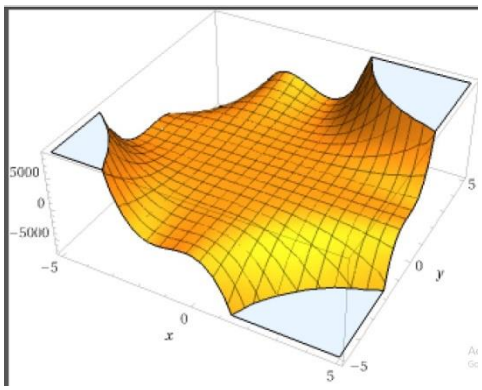
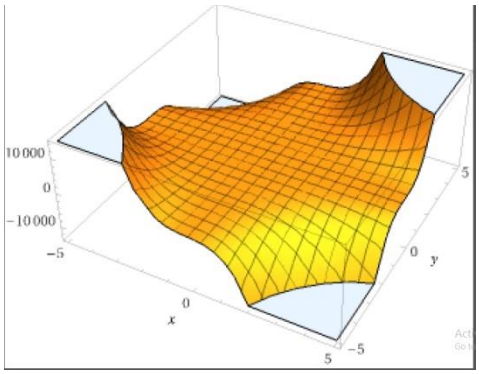
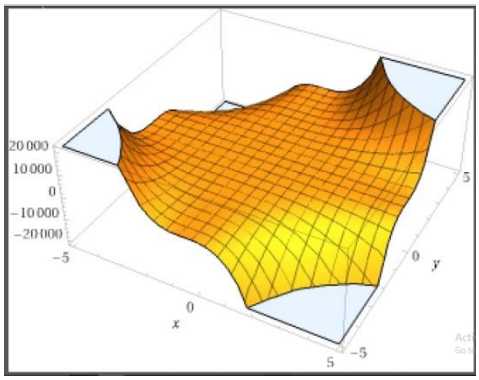
Lopinavir (L)	M (G, x, y) = $8xy^3$ + $14x^2y^2 + 20x^2y^3 + 7x^3y^3$.	
Ritonavir (Ri)	M (G, x, y) = $8xy^3$ + $14x^2y^2 + 20x^2y^3 + 7x^3y^3$.	
Arbidol (A)	M (G, x, y) = xy^2+6xy^3+ $6x^2y^2 + 9x^2y^3 + 9x^3y^3$.	
Theaflavin (Th)	M (G, x, y) = $10xy^3 + 22x^2y^3 + 14x^3y^3$.	

Table 3. Physicochemical properties of Antiviral drugs used in Covid-19 treatment

DRUGS	BP	E	FP	MR	PSA	P	T	MV	IC50
C	460.6	72.1	232.3	97.4	28	38.6	44	287.9	1.38
HC	516.7	83	266.3	99	48	39.2	49.8	285.4	0.72
Re				149.5	213	59.3	62.3	409	0.987
L	924.2	140.8	512.7	179.2	120	71	49.5	540.5	5.25
Ri	947	144.4	526.6	198.9	202	78.9	53.7	581.7	8.63
A	591.8	91.5	311.7	121.9	80	48.3	45.3	347.3	3.54
Th	1003.9	153.5	336.5	137.3	218	54.4	138.6	301	8.44

Table 4. The values of topological indices of the molecular structures of antiviral drugs used in the treatment of Covid-19

	SO	SO_r	SO_w	SO_{rw}	Z1
C	76.69	45.56	181.26	63.63	106
HC	79.52	46.97	186.92	65.05	110
Re	157.81	98.86	401.09	156.95	216
L	166.71	100.32	399.17	142.48	230
Ri	166.71	100.32	399.17	142.48	230
A	108.81	67.07	270.92	102.08	150
Th	170.34	108.79	439.74	172.99	234

Table 3 displays the benchmark sets of the physicochemical characteristics of the medications used to treat COVID-19 patients, including chloroquine, hydroxychloroquine, remdesivir, lopinavir, ritonavir, arbidol, theaflavin, and thalidomide [27]. These characteristics include polar surface area (PSA), polarizability (P), surface tension (T), molar volume (MV), enthalpy of vaporization (E), flash point (FP), molar refractivity (MR), and boiling point (BP).

Table 4 represents the values of the topological indices $SO, SO_r, SO_w, SO_{rw}, and Z_1$ corresponding to each of the antiviral drugs.

Curvilinear regression analysis is used to fit curves [1]. Here, linear, quadratic, and cubic curves are fitted to the data.$y = a + bx; y = a + bx + cx^2; y = a + bx + cx^2 + dx^3$ be the linear, quadratic and cubic curve fitted for the data, where y represents the dependant variable — the physicochemical properties, and x represents the independent variable — the selected indices. The correlation coefficient R and its square R^2 is evaluated to predict the model.

Table 5 displays the correlation between the physicochemical characteristics and topological indices of medications used to treat COVID-19 in a linear regression model. The correlation coefficient R and the best linear curve fitted to the data are shown in Table 8.

Table 6 displays the correlation between the physicochemical characteristics and topological indices of medications used to treat COVID-19 in a quadratic regression model. The correlation coefficient R and the best quadratic curve fitted to the data are shown in Table 9. Table 7 displays the relationship between the topological indices and physicochemical characteristics of different medications used to treat COVID-19 in a cubic regression model. The correlation coefficient R and the best cubic curve fitted to the data are shown in Table 10.

Table 5. The correlation coefficient (R) squared between topological indices and the physicochemical characteristics of several medications used to treat COVID-19, as determined by the linear regression model

	SO	SO_r	SO_w	SO_{rw}	Z1
BP	0.982048	**0.983**	0.9798	0.9486	0.9814
E	0.9751	**0.9769**	0.9737	0.9437	0.9745
FP	0.6831	0.6068	0.5857	0.463	**0.6886**
MR	0.7383	0.6675	0.6454	0.523	**0.7447**
PSA	0.8179	0.8505	0.8603	**0.8888**	0.8123
P	0.738	0.6673	0.6452	0.5229	**0.7444**
T	0.2418	0.2996	0.3119	**0.3895**	0.2385
MV	0.4489	0.3716	0.35	0.2389	**0.4559**
IC50	0.5141	0.5023	0.4886	0.4304	**0.5209**

Table 6. The correlation coefficient (R) squared between topological indices and the physicochemical characteristics of several medications used to treat COVID-19, as determined by the quadratic regression model

	SO	SO_r	SO_w	SO_{rw}	Z1
BP	**0.9916**	0.9912	0.9868	0.9488	0.9906
E	0.9869	**0.9876**	0.9831	0.9437	0.9856
FP	0.6876	0.6838	0.6869	0.7255	**0.6911**
MR	0.7386	0.7132	0.7131	0.7421	**0.7447**
PSA	0.8182	0.8551	0.8684	**0.895**	0.8134
P	0.7383	0.7131	0.713	0.7419	**0.7444**
T	0.3317	0.6055	0.6589	**0.8155**	0.3147
MV	0.4522	0.4855	0.5087	**0.6435**	0.4569
IC50	0.5498	0.5214	0.4979	0.435	**0.5625**

Table 7. The correlation coefficient (R) squared between topological indices and the physicochemical characteristics of several medications used to treat COVID-19, as determined by the cubic regression model

	SO	SO_r	SO_w	SO_{rw}	Z1
BP	0.9974	0.994	0.9936	0.9926	**0.9981**
E	0.9951	0.9898	0.9893	0.988	**0.9964**
FP	0.9386	0.9833	0.9841	**0.9878**	0.9184
MR	0.7447	0.8419	0.8658	**0.8958**	0.7463
PSA	0.8295	0.8553	0.8686	**0.901**	0.8318
P	0.7446	0.8423	0.8662	**0.896**	0.7461
T	0.4992	0.9606	**0.9923**	0.9672	0.4266
MV	0.4842	0.7753	0.8324	**0.9135**	0.4706
IC50	0.871	0.6142	0.5569	0.4588	**0.8855**

Table 8. List the most compatible linear regression model fitting curves for predicting the physicochemical properties of various drugs used to treat COVID-19 patients.

Linear Curve	R
$BP = 8.4506 * SO_r + 80.106$	0.9914635646
$E = 1.2405 * SO_r + 17.246$	0.988382517
$PSA = 1.7334 * SO_{RW} - 79.548$	0.9427619
$T = 0.477 * SO_{rw} + 5.692$	0.6240993511
$FP = 1.6858 * Z1 + 66.532$	0.8298192574
$MR = 0.5701 * Z1 + 36.537$	0.8629600222
$MV = 1.4226 * Z1 + 133.94$	0.675203673
$IC50 = 0.0421 * Z1 - 3.5336$	0.721734023

Table 9: List the most compatible quadratic regression model fitting curves for predicting the physicochemical properties of various drugs used to treat COVID-19 patients.

Quadratic Curve	R
$BP = 0.0322 * SO^2 - 2.6863 * SO + 501.27$	0.9957911428
$E = 0.0106SO_r^2 - 0.3689SO_r + 71.355$	0.9937806599
$PSA = 0.0054SO_{rw}^2 + 0.4977SO_{rw} - 18.357$	0.9460443964
$T = 0.0186SO_{rw}^2 - 3.776SO_{rw} + 216.31$	0.9030503862
$MV = -0.0662SO_{rw}^2 + 16.471SO_{rw} - 519.48$	0.8021845174
$FP = -0.0045Z1^2 + 3.247Z1 - 53.221$	0.8313242448
$MR = -4E - 05Z1^2 + 0.5822Z1 + 35.607$	0.8629600222
$P = -2E - 05Z1^2 + 0.2323Z1 + 13.966$	0.8627861844
$IC50 = 0.0005Z1^2 - 0.1341Z1 + 9.9581$	0.75

Table 10. List the most compatible cubic regression model fitting curves for predicting the physicochemical properties of various drugs used to treat COVID-19 patients.

Cubic Curve	R
$T = 5E - 05SO_w^3 - 0.0381SO_w^2 + 10.244SO_w - 827.8$	0.9961425601
$FP = -0.0018SO_{rw}^3 + 0.607SO_{rw}^2 - 60.683SO_{rw} + 2126.6$	0.9938812806
$MR = -0.0004SO_{rw}^3 + 0.1448SO_{rw}^2 - 13.923SO_{rw} + 512.61$	0.9464671151
$PSA = -0.0002SO_{rw}^3 + 0.0719SO_{rw}^2 - 6.988SO_{rw} + 239.36$	0.949210198
$P = -0.0002SO_{rw}^3 + 0.0576SO_{rw}^2 - 5.5357SO_{rw} + 203.72$	0.9465727653
$MV = -0.0019SO_{rw}^3 + 0.6106SO_{rw}^2 - 59.784SO_{rw} + 2105.8$	0.9557719393
$BP = 0.0013Z1^3 - 0.6182Z1^2 + 96.762Z1 - 4382.8$	0.9990495483
$E = 0.0002Z1^3 - 0.1086Z1^2 + 16.924Z1 - 769.81$	0.9981983771
$IC50 = 5E - 05Z1^3 - 0.0235Z1^2 + 3.696Z1 - 184.41$	0.9410100956

4. Conclusion

Research indicates that various Sombor indices studied here demonstrate significant potential in predicting antiviral drugs' physicochemical properties in COVID-19 treatment. The models were analyzed using seven descriptors and five topological indices. An analysis has been done for the Quantitative Structure-Property Relationship (QSPR) of the antiviral drugs through curvilinear regression models —including linear, quadratic, and cubic regression—revealed the following insights:

In the linear regression model, the most effective predictive topological indices were identified as

- SO_r for the physicochemical properties of BP and E
- SO_{rw} for the physicochemical properties of PSA and T
- Z1 for the physicochemical properties FP, MR, MV and IC50

In the quadratic regression model, the most effective predictive topological indices were identified as

- So, for the physicochemical properties, BP
- SO_r for the physicochemical properties, E
- SO_{rw} for the physicochemical properties of PSA, T and MV
- Z1 for the physicochemical properties FP, MR, P and IC50

In the cubic regression model, the most effective predictive topological indices were identified as

- SO_w for the physicochemical properties, T
- SO_{rw} for the physicochemical properties FP, MR, PSA, P, MV
- Z1 for the physicochemical properties BP, E, and IC50

Figures 2,3,4 and 5 show the Plot of linear, quadratic and cubic regression equations of the various physicochemical properties, which are the best-predicted pair according to our analysis.

Data Availability Statement

The data on the physicochemical properties and the structure of the drugs used in this study was taken from the site *datahttps://pubchem.ncbi.nlm.nih.gov/docs/structure-search*. Also, the 3D Plot was done using the tool site *https://www.wolframalpha.com/*

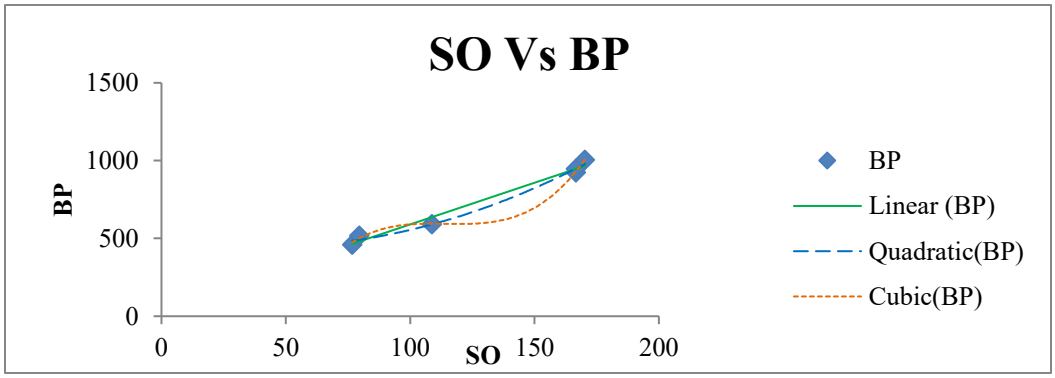
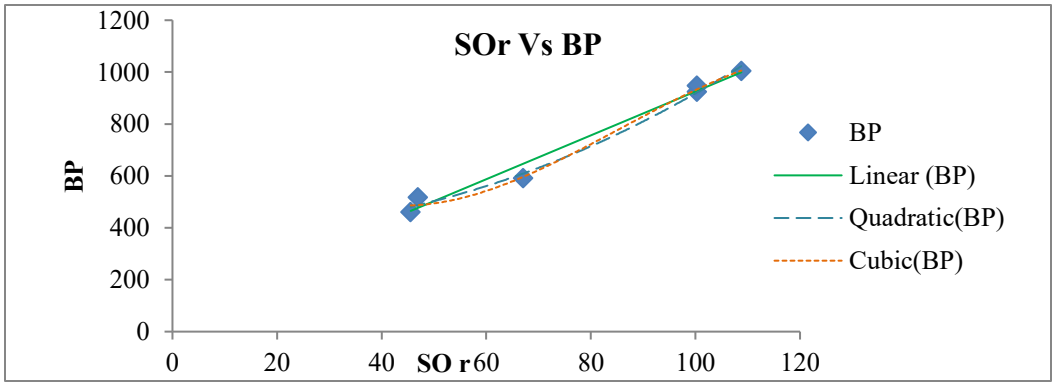


Fig. 2 Plot of curvilinear regression equations of Sombor index with Boiling Point



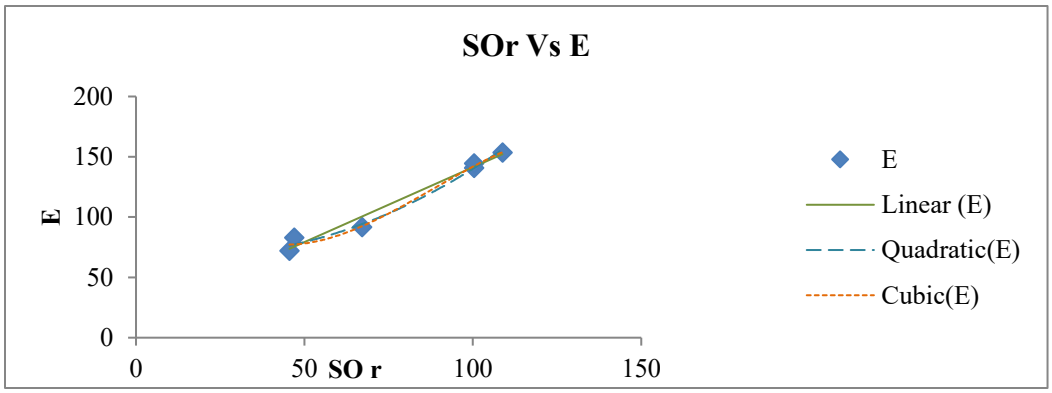
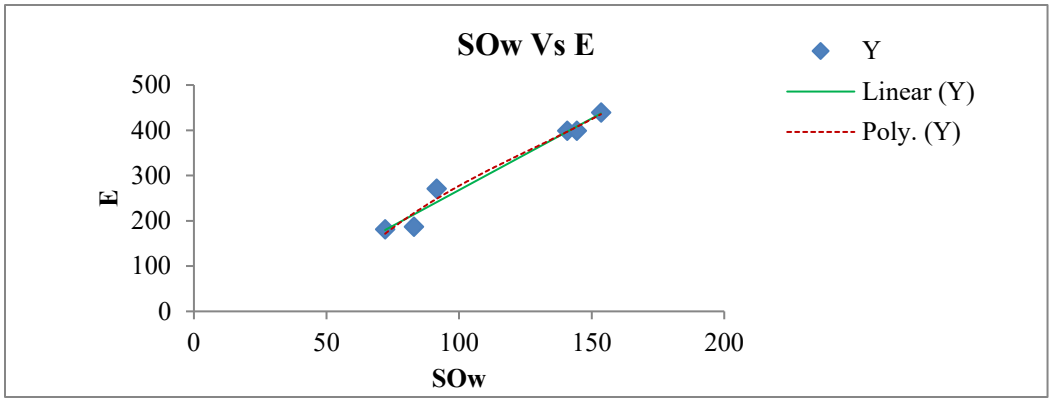


Fig. 3 Plot of curvilinear regression equations of Reduced Sombor index with Boiling Point and Enthalpy of Vaporization.



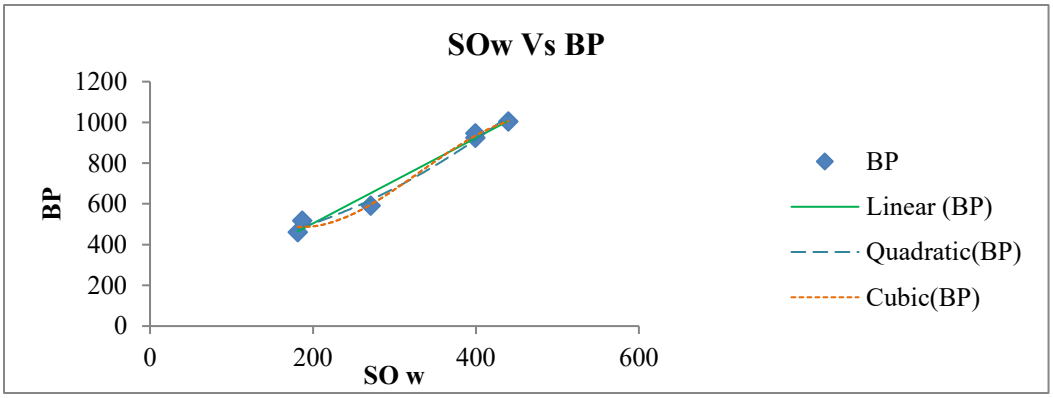
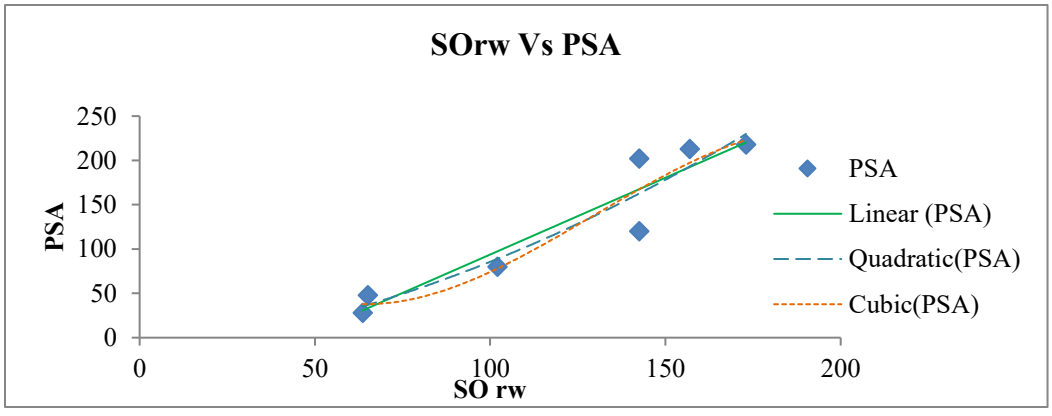


Fig. 4 Plot of curvilinear regression equations of Weighted Sombor index with Boiling Point and Enthalpy of Vaporization.



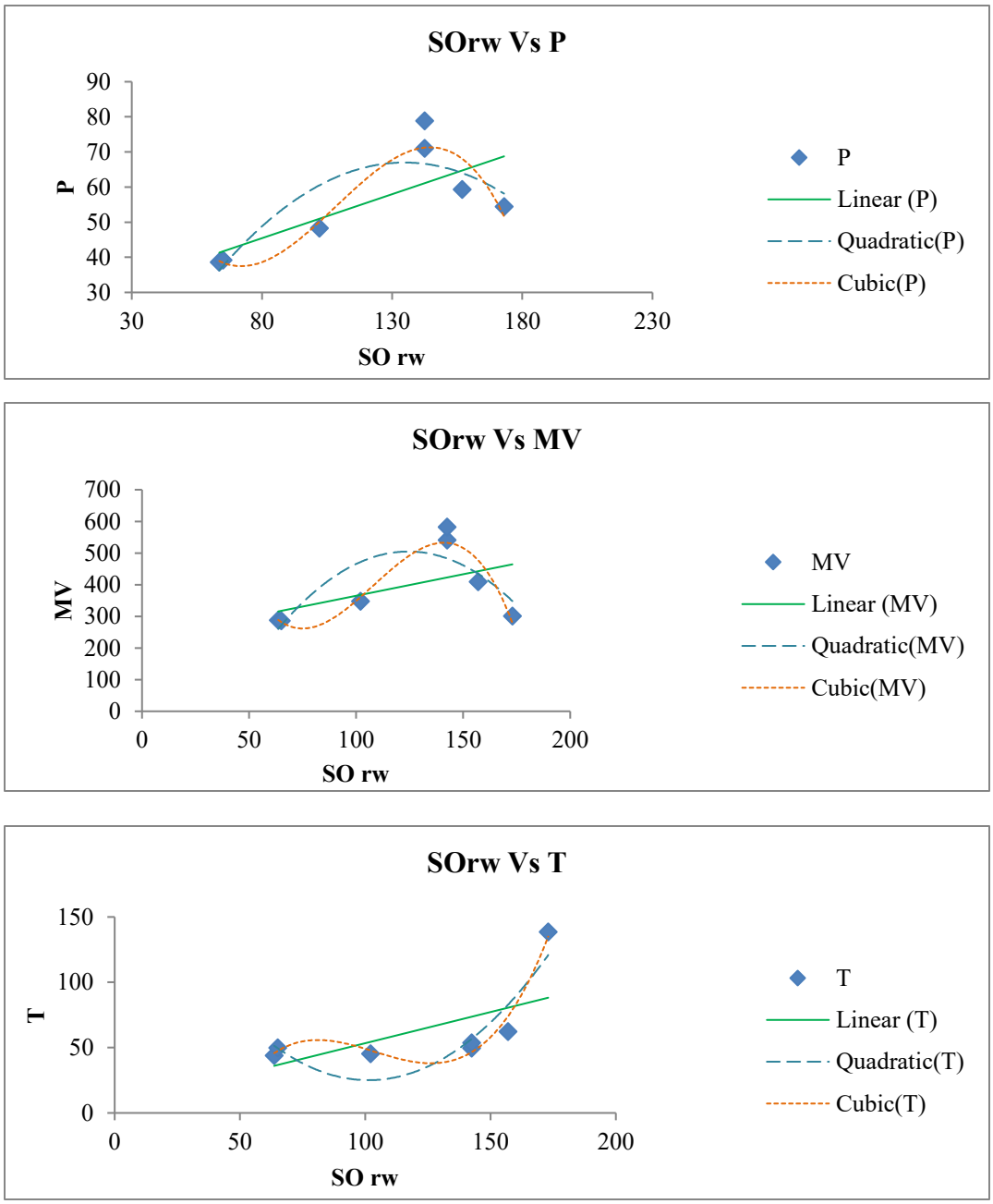


Fig. 5 Plot of curvilinear regression equations of Reduced Weighted Sombor index with Polar Surface Area, Polarizability, Surface Tension and Molar Volume

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