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ON MASS SOMBOR AND REVERSE MASS SOMBOR INDICES WITH APPLICATIONS TO ANTI-ASTHMATIC DRUGS

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Abstract. The Sombor index and reverse Sombor index are well-known degree-based topological descriptors with applications in chemical graph theory and quantitative structure–property relationship (QSPR) studies. Motivated by mass-based graph descriptors, we introduce the mass Sombor index $MSO(G)$ and the reverse mass Sombor index $RMSO(G)$. Closed-form expressions for these indices are derived for several standard graphs, including cycles, complete graphs, wheel graphs, regular graphs, and paths. The derivations are obtained by considering the mass distribution of the vertices and appropriate edge partitions of the corresponding graphs. Furthermore, the chemical applicability of the mass Sombor index is investigated through correlation and regression analyses of selected anti-asthmatic drugs using their physicochemical properties. The results indicate that the mass Sombor index exhibits significant correlations with several physicochemical properties of the considered anti-asthmatic drugs, demonstrating its potential as a useful molecular descriptor in QSPR studies.

1. Introduction

Asthma is a chronic respiratory disorder characterized by airway inflammation, increased mucus production, and narrowing of the airways, which can cause difficulty in breathing. Since asthma is a long-term condition, many patients require continuous medication for symptom control. Despite advances in treatment, uncontrolled symptoms and acute attacks remain significant clinical and public-health concerns.

The complex nature of asthma has led to the development of various anti-asthmatic drugs. Leukotriene receptor antagonists, such as Montelukast, Pranlukast, and Zafirlukast, help reduce airway inflammation and narrowing, while bronchodilator drugs, including Salmeterol, Formoterol, Indacaterol, Olodaterol, and Vilanterol, improve airflow by relaxing the airway muscles. The study of the molecular structure and physicochemical properties of these drugs is therefore of considerable interest.

Chemical graph theory provides useful mathematical tools for representing molecular structures, where atoms are treated as vertices and chemical bonds as edges.

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Topological indices derived from molecular graphs serve as numerical descriptors and are widely used in quantitative structure–property relationship (QSPR) studies.

Motivated by mass-based graph descriptors [1,5], the Mass Sombor index $MSO(G)$ and the Reverse Mass Sombor index $RMSO(G)$ are introduced in this work. Closed-form expressions for both indices are obtained for several standard graph families, including paths, cycles, complete graphs, and wheel graphs.

The chemical applicability of $MSO(G)$ is further investigated through QSPR analysis of selected anti-asthmatic drugs. The results demonstrate the potential of the Mass Sombor index as a molecular descriptor for characterizing the physicochemical properties of anti-asthmatic drugs.

2. Preliminaries

A graph is said to be simple if it contains neither multiple edges nor loops. Throughout this paper, we consider finite, simple, connected, and undirected graphs. Let $G = (V, E)$ be a graph with vertex set V and edge set E. The order and size of G are denoted by $|V| = n$ and $|E| = m$, respectively. For a vertex $u \in V(G)$, the degree of u, denoted by $d(v)$, is the number of edges incident with u. The degree of an edge $e = uv$ is defined by $d(e) = d(u) + d(v) - 2$.

For any unexplained notation or terminology, the reader is referred to [4].

Definition 2.1. [3] Let $w_1, w_2, \ldots, w_n$ be the mass of the vertices $u_1, u_2, \ldots, u_n$. Then the mass of a vertex u_ℓ is defined as

$$w(u_\ell) = d(u_\ell), \ell = 1, 2, , n$$

.

Definition 2.2. [3] Let $e_1, e_2, \ldots, e_n$ be the edges of a graph G. Then the edge mass of $e = uv$ is defined as

$$w(e) = d(u) + d(v) - 2$$

Definition 2.3. [3] For a vertex $u \in G$, the mass degree of u is defined as

$$d^w(u) = \sum_{e=uv} w(e)$$

Definition 2.4. [2] The Sombor index of a graph G is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2},$$

where $d(u)$ is the degree of the vertex $u \in G$.

Definition 2.5. [7] The reverse Sombor index of a graph G, denoted by $R_eSO(G)$, is defined as

$$\begin{aligned} R_eSO(G) &= \sum_{uv\in E(G)} \sqrt{c(u)^2 + c(v)^2} \\ &= \sum_{uv\in E(G)} \sqrt{[\Delta(G) - d(u) + 1]^2 + [\Delta(G) - d(v) + 1]^2}, \end{aligned}$$

where $d(u)$ is the degree of the vertex u of G and $c(u) = \Delta - d(u) + 1$ is the reverse vertex degree of u.

Motivated by the concept of the Mass version of the first and second Zagreb indices [3] and the reverse Sombor index [7], we introduce new mass-based topological descriptors called the mass Sombor index and reverse mass Sombor index of a graph.

Definition 2.6. The mass Sombor index of a graph G denoted by $MSO(G)$ and is defined as

$$MSO(G) = \sum_{uv\in E(G)} \sqrt{d^w(u)^2 + d^w(v)^2}$$

where $d^w(u)$ is the mass degree of the vertex u.

Definition 2.7. The reverse mass Sombor index of a graph G, denoted by $RMSO(G)$, is defined as

$$\begin{aligned} RMSO(G) &= \sum_{uv\in E(G)} \sqrt{c^w(u)^2 + c^w(v)^2} \\ &= \sum_{uv\in E(G)} \sqrt{[\Delta^w(G) - d^w(u) + 1]^2 + [\Delta^w(G) - d^w(v) + 1]^2}, \end{aligned}$$

where $d^w(u)$ is the mass degree, $c^w(u) = \Delta^w(G) - d^w(u) + 1$ is the reverse mass vertex degree and $\Delta^w(G)$ is the maximum mass degree of a graph G.

3. Main Results

In this section, we derive closed-form expressions for the mass Sombor index and the reverse mass Sombor index of the cycle graph (C_n), complete graph (K_n), wheel graph (W_n), and path graph (P_n), respectively. For each graph, the vertex masses and corresponding degrees are determined, and the edge contributions are evaluated accordingly. These results are then used to obtain explicit formulae for the mass Sombor index and the reverse mass Sombor index. The obtained closed-form expressions provide exact values of these mass-based Sombor indices for the considered standard graph families and serve as a basis for further investigations of their structural and chemical applications.

Theorem 3.1. *Let C_n be a cycle graph of order n, where $n \geq 3$. Then the mass Sombor index of C_n is $MSO(C_n) = 4n\sqrt{2}$.*

Proof. Let C_n be the cycle graph with vertex set

$$V(C_n) = \{u_1, u_2, \ldots, u_n\}.$$

Since C_n is a 2-regular graph, we have $d(u_\ell) = 2, 1 \leq \ell \leq n$. For an edge $e = u_\ell u_{\ell+1} \in E(C_n)$, the edge mass is defined by

$$w(e) = d(u_\ell) + d(u_{\ell+1}) - 2.$$

Since $d(u_\ell) = d(u_{\ell+1}) = 2$, we obtain

$$w(e) = 2 + 2 - 2 = 2.$$

Each vertex of C_n is incident with exactly two edges. Therefore, the mass degree of every vertex is

$$d^w(u_\ell) = 2 + 2 = 4.$$

By the definition of the mass Sombor index,

$$MSO(G) = \sum_{uv \in E(C_n)} \sqrt{d^w(u)^2 + d^w(v)^2},$$

we obtain

$$\begin{aligned} MSO(C_n) &= \sum_{u_\ell u_{\ell+1} \in E(C_n)} \sqrt{d^w(u_\ell)^2 + d^w(u_{\ell+1})^2} \\ &= \sum_{u_\ell u_{\ell+1} \in E(C_n)} \sqrt{4^2 + 4^2} \\ &= n\sqrt{16 + 16} = 4n\sqrt{2}. \end{aligned}$$

Theorem 3.2. *Let C_n be a cycle graph of order n, where $n \geq 3$. Then the reverse mass Sombor index of C_n is $RMSO(C_n) = n\sqrt{2}$.*

Proof. Let C_n be the cycle graph with vertex set

$$V(C_n) = \{u_1, u_2, \ldots, u_n\}.$$

Since C_n is a 2-regular graph, we have $d(u_\ell) = 2, 1 \leq \ell \leq n$. For an edge $e = u_\ell u_{\ell+1} \in E(C_n)$, the edge mass is defined by

$$w(e) = d(u_\ell) + d(u_{\ell+1}) - 2.$$

Since $d(u_\ell) = d(u_{\ell+1}) = 2$, we obtain

$$w(e) = 2 + 2 - 2 = 2.$$

Each vertex of C_n is incident with exactly two edges. Therefore, the mass degree of every vertex is

$$d^w(u_\ell) = 2 + 2 = 4.$$

Thus every vertex of C_n has mass degree 4. Consequently, the maximum mass degree of C_n is $\Delta^w(C_n) = 4$. By the definition of the reverse mass Sombor index,

$$RMSO(G) = \sum_{uv \in E(C_n)} \sqrt{[\Delta^w(G) - d^w(u) + 1]^2 + [\Delta^w(G) - d^w(v) + 1]^2},$$

we obtain

$$\begin{aligned} RMSO(C_n) &= \sum_{u_\ell u_{\ell+1}\in E(C_n)} \sqrt{[\Delta^w(C_n) - d^w(u_\ell) + 1]^2 + [\Delta^w(C_n) - d^w(u_{\ell+1}) + 1]^2} \\ &= \sum_{u_\ell u_{\ell+1}\in E(C_n)} \sqrt{(4-4+1)^2 + (4-4+1)^2} \\ &= n\sqrt{2}. \end{aligned}$$

Theorem 3.3. *Let K_n be a complete graph of order n, where $n \geq 2$. Then the mass Sombor index of K_n is*

$$MSO(K_n) = n(n-1)^2(n-2)\sqrt{2}.$$

Proof. Let K_n be the complete graph with vertex set

$$V(K_n) = \{u_1, u_2, \ldots, u_n\}.$$

Since K_n is an $(n-1)$-regular graph, we have

$$d(u_\ell) = n-1,\ 1 \leq \ell \leq n.$$

For every edge $e = u_iu_j \in E(K_n)$, the edge mass is defined by

$$w(e) = d(u_i) + d(u_j) - 2.$$

Since $d(u_i) = d(u_j) = n-1$, we obtain

$$w(e) = (n-1) + (n-1) - 2 = 2(n-2).$$

Each vertex of K_n is incident with exactly $n-1$ edges. Hence, the mass degree of every vertex is

$$d^w(u_\ell) = (n-1)\cdot 2(n-2) = 2(n-1)(n-2).$$

By the definition of the mass Sombor index,

$$\begin{aligned} MSO(K_n) &= \sum_{u_iu_j\in E(K_n)} \sqrt{d^w(u_i)^2 + d^w(u_j)^2} \\ &= \sum_{u_iu_j\in E(K_n)} \sqrt{[2(n-1)(n-2)]^2 + [2(n-1)(n-2)]^2} \\ &= |E(K_n)|\, 2(n-1)(n-2)\sqrt{2} \\ &= \frac{n(n-1)}{2}\cdot 2(n-1)(n-2)\sqrt{2} \\ &= n(n-1)^2(n-2)\sqrt{2}. \end{aligned}$$

Theorem 3.4. *Let K_n be a complete graph of order n, where $n \geq 2$. Then the reverse mass Sombor index of K_n is*

$$RMSO(K_n) = \frac{n(n-1)}{\sqrt{2}}.$$

Proof. Let K_n be the complete graph with vertex set

$$V(K_n) = \{u_1, u_2, \ldots, u_n\}.$$

Since K_n is an $(n-1)$-regular graph, we have

$$d(u_\ell) = n-1, \qquad 1 \leq \ell \leq n.$$

For every edge $e = u_i u_j \in E(K_n)$, the edge mass is defined by

$$w(e) = d(u_i) + d(u_j) - 2.$$

Since $d(u_i) = d(u_j) = n-1$, we obtain

$$w(e) = (n-1) + (n-1) - 2 = 2(n-2).$$

Each vertex of K_n is incident with exactly $n-1$ edges. Hence, the mass degree of every vertex is

$$d^w(u_\ell) = (n-1) \cdot 2(n-2) = 2(n-1)(n-2).$$

Since $d^w(u_\ell) = \Delta_w(K_n) = 2(n-1)(n-2)$, we have

$$c^w(u) = \Delta^w - d^w(u_\ell) + 1 = 1$$

By the definition of the reverse mass Sombor index,

$$\begin{aligned} RMSO(K_n) &= \sum_{u_i u_j \in E(K_n)} \sqrt{1^2 + 1^2} \\ &= \frac{n(n-1)}{2} \cdot \sqrt{2} \\ &= \frac{n(n-1)}{\sqrt{2}}. \end{aligned}$$

Theorem 3.5. *Let $K_{1,n-1}$ be the star graph of order n, where $n \geq 2$. Then the mass Sombor index of $K_{1,n-1}$ is*

$$MSO(K_{1,n-1}) = (n-1)(n-2)\sqrt{n^2 - 2n + 2}$$

Proof. Let $K_{1,n-1}$ be the star graph with central vertex u_0 and leaf vertices $\{u_1, u_2, \ldots, u_{n-1}\}$. The edge set of $K_{1,n-1}$ is given by

$$E(K_{1,n-1}) = \{u_0 u_\ell : 1 \leq \ell \leq n-1\}.$$

Since u_0 is adjacent to all the $n-1$ leaf vertices, $d(u_0) = n-1$ and $d(u_\ell) = 1$, $1 \leq \ell \leq n-1$
For every edge $e = u_0 u_\ell \in E(K_{1,n-1})$, the edge mass is

$$w(e) = d(u_0) + d(u_\ell) - 2 = (n-1) + 1 - 2 = n-2.$$

Since $K_{1,n-1}$ consists of $n-1$ edges, the mass degree of the central vertex is

$$d^w(u_0) = \sum_{\ell=1}^{n-1} w(u_0 u_\ell) = (n-1)(n-2).$$

For each leaf vertex u_ℓ, $1 \leq \ell \leq n-1$, we have $d^w(u_\ell) = (n-2)$.
Therefore, by the definition of the mass Sombor index,

$$\begin{aligned} MSO(K_{1,n-1}) &= \sum_{u_0u_\ell \in E(K_{1,n-1})} \sqrt{d^w(u_0)^2 + d^w(u_\ell)^2} \\ &= (n-1)\sqrt{[(n-1)(n-2)]^2 + (n-2)^2} \\ &= (n-1)(n-2)\sqrt{(n-1)^2+1} \\ &= (n-1)(n-2)\sqrt{n^2-2n+2}. \end{aligned}$$

Theorem 3.6. *Let $K_{1,n-1}$ be the star graph of order n, where $n \geq 2$. Then the reverse mass Sombor index of $K_{1,n-1}$ is*

$$RMSO(K_{1,n-1}) = (n-1)\sqrt{1+(n^2-4n+5)^2}$$

Proof. Let $K_{1,n-1}$ be the star graph with central vertex u_0 and leaf vertices $\{u_1, u_2, \ldots, u_{n-1}\}$.
The edge set of $K_{1,n-1}$ is given by

$$E(K_{1,n-1}) = \{u_0u_\ell : 1 \leq \ell \leq n-1\}.$$

Since u_0 is adjacent to all the $n-1$ leaf vertices, $d(u_0) = n-1$ and $d(u_\ell) = 1$, $1 \leq \ell \leq n-1$
For every edge $e = u_0u_\ell \in E(K_{1,n-1})$, the edge mass is

$$w(e) = d(u_0) + d(u_\ell) - 2 = (n-1) + 1 - 2 = n-2.$$

Since $K_{1,n-1}$ consists of $n-1$ edges, the mass degree of the central vertex is

$$d^w(u_0) = \sum_{\ell=1}^{n-1} w(u_0u_\ell) = (n-1)(n-2).$$

For each leaf vertex u_ℓ, $1 \leq \ell \leq n-1$, we have $d^w(u_\ell) = (n-2)$.
Therefore, the maximum mass degree of $K_{1,n-1}$ is

$$\Delta^w(K_{1,n-1}) = (n-1)(n-2).$$

By the definition of the reverse mass Sombor index,

$$\begin{aligned} RMSO(K_{1,n-1}) &= \sum_{u_0u_\ell \in E(K_{1,n-1})} \sqrt{[\Delta^w - d^w(u_0) + 1]^2 + [\Delta^w - d^w(u_\ell) + 1]^2} \\ &= (n-1)\sqrt{[(n-1)(n-2) - (n-1)(n-2) + 1]^2 + [(n-1)(n-2) - (n-2) + 1]^2} \\ &= (n-1)\sqrt{1 + [(n-1)(n-2) - (n-2) + 1]^2} \\ &= (n-1)\sqrt{1 + [(n-2)^2 + 1]^2} \\ &= (n-1)\sqrt{1 + (n^2-4n+5)^2}. \end{aligned}$$

Theorem 3.7. *Let W_n be a wheel graph of order n, where $n \geq 4$. Then the mass Sombor index of W_n is*

$$MSO(W_n) = (n-1)\left[\sqrt{n^2(n-1)^2 + (n+8)^2} + (n+8)\sqrt{2}\right].$$

Proof. Let W_n be the wheel graph with vertex set

$$V(W_n) = \{u_0, u_1, u_2, \ldots, u_{n-1}\},$$

where u_0 is the central vertex and $u_1, u_2, \ldots, u_{n-1}$ are the rim vertices of the cycle C_{n-1}.
Since u_0 is adjacent to all the $n-1$ rim vertices, $d(u_0) = n-1$.
Each rim vertex u_ℓ is adjacent to the central vertex u_0 and two adjacent rim vertices. Hence,

$$d(u_\ell) = 3,\ 1 \leq \ell \leq n-1.$$

For every edge $e = u_\ell u_{\ell+1} \in E(W_n)$, the edge mass is defined by

$$w(e) = d(u_\ell) + d(u_{\ell+1}) - 2.$$

For every spoke edge $u_0u_\ell, w(u_0u_\ell) = (n-1) + 3 - 2 = n$.
Since (u_0) is incident with $(n-1)$ spoke edges, its mass degree is $d^w(u_0) = (n-1)n$.
For every rim edge $u_\ell u_{\ell+1}$ of C_{n-1}, we have

$$w(u_\ell u_{\ell+1}) = 3 + 3 - 2 = 4.$$

Therefore, each rim vertex u_ℓ is incident with one spoke edge of mass n and two rim edges of mass 4. Hence

$$d^w(u_\ell) = n + 4 + 4 = n + 8,\ 1 \leq \ell \leq n-1.$$

The wheel graph W_n consists of $n-1$ spoke edges and $n-1$ rim edges.
Thus, by the definition of the mass Sombor index,

$$\begin{aligned} MSO(W_n) &= \sum_{u_0u_\ell \in E(W_n)} \sqrt{d^w(u_0)^2 + d^w(u_\ell)^2} + \sum_{u_\ell u_{\ell+1} \in E(W_n)} \sqrt{d^w(u_\ell)^2 + d^w(u_{\ell+1})^2} \\ &= (n-1)\sqrt{[n(n-1)]^2 + (n+8)^2} + (n-1)\sqrt{(n+8)^2 + (n+8)^2} \\ &= (n-1)[\sqrt{[n(n-1)]^2 + (n+8)^2} + (n+8)\sqrt{2}]. \end{aligned}$$

Theorem 3.8. *Let W_n be a wheel graph of order n, where $n \geq 4$. Then the mass Sombor index of W_n is*

$$MSO(W_n) = (n-1)\left[\sqrt{n^2(n-1)^2 + (n+8)^2} + (n+8)\sqrt{2}\right].$$

Proof. Let W_n be the wheel graph with vertex set

$$V(W_n) = \{u_0, u_1, u_2, \ldots, u_{n-1}\},$$

where u_0 is the central vertex and $\{u_1, u_2, \ldots, u_{n-1}\}$ are the rim vertices of the cycle C_{n-1}.
Since u_0 is adjacent to all the $n-1$ rim vertices, $d(u_0) = n-1$.
Each rim vertex u_ℓ is adjacent to the central vertex u_0 and two adjacent rim vertices. Hence,

$$d(u_\ell) = 3,\ 1 \leq \ell \leq n-1.$$

For every edge $e = u_\ell u_{\ell+1} \in E(W_n)$, the edge mass is defined by

$$w(e) = d(u_\ell) + d(u_{\ell+1}) - 2.$$

For every spoke edge $u_0u_\ell, w(u_0u_\ell) = (n-1) + 3 - 2 = n$.
Since (u_0) is incident with $(n-1)$ spoke edges, its mass degree is $d^w(u_0) = (n-1)n$.
For every rim edge $u_\ell u_{\ell+1}$ of C_{n-1}, we have

$$w(u_\ell u_{\ell+1}) = 3 + 3 - 2 = 4.$$

Therefore,each rim vertex u_ℓ is incident with one spoke edge of mass n and two rim edges of mass 4. Hence

$$d^w(u_\ell) = n + 4 + 4 = n + 8,\ 1 \le \ell \le n-1.$$

Consequently,

$$\Delta^w(W_n) = \max\{n(n-1),\ n+8\}.$$

For $n \ge 4$,

$$n(n-1) \ge n + 8$$

with equality when $n = 4$. Thus,

$$\Delta^w(W_n) = n(n-1).$$

The reverse mass degree of a vertex u is

$$c^w(u) = \Delta^w(W_n) - d^w(u) + 1.$$

Therefore,

$$c^w(u_0) = n(n-1) - n(n-1) + 1 = 1,$$

while, for every rim vertex u_ℓ,

$$\begin{aligned} c^w(u_\ell) &= n(n-1) - (n+8) + 1 \\ &= n^2 - n - n - 8 + 1 \\ &= n^2 - 2n - 7. \end{aligned}$$

The wheel graph W_n consists of $n-1$ spoke edges and $n-1$ rim edges. Hence, by the definition of the reverse mass Sombor index,

$$RMSO(W_n) = \sum_{u_0u_\ell \in E(W_n)} \sqrt{c^w(u_0)^2 + c^w(u_\ell)^2} + \sum_{u_\ell u_{\ell+1} \in E(W_n)} \sqrt{c^w(u_\ell)^2 + c^w(u_{\ell+1})^2}.$$

Since there are $n-1$ spoke edges and $n-1$ rim edges,

$$\begin{aligned} RMSO(W_n) &= (n-1)\sqrt{1^2 + (n^2-2n-7)^2} + (n-1)\sqrt{(n^2-2n-7)^2 + (n^2-2n-7)^2} \\ &= (n-1)\left[\sqrt{1 + (n^2-2n-7)^2} + (n^2-2n-7)\sqrt{2}\right]. \end{aligned}$$

□

Theorem 3.9. *Let G be an r-regular graph of order n, where $n \ge 2$. Then the mass Sombor index of $r-regular$ is*

$$MSO(r-regular) = 2nr^2(r-1).$$

Proof. Let G be an r-regular graph of order n. Then, for every vertex $u \in V(G)$, $d(u) = r$
For each $uv \in E(G)$, the edge mass is $w(uv) = d(u) + d(v) - 2$.
Since G is r-regular, $w(uv) = r + r - 2 = 2r(r-1)$. Every vertex is incident with r edges. Therefore, the mass degree of every vertex $u \in V(G)$ is

$$d^w(u) = r \cdot 2(r-1) = 2r(r-1).$$

Since G is r-regular of order n, by the handshaking Lemma,

$$|E(G) = \frac{nr}{2}.$$

By the definition of the mass Sombor index,

$$\begin{aligned} MSO(r-regular) &= \sum_{uv \in E(r-regular)} \sqrt{[2r(r-1)]^2 + [2r(r-1)]^2} \\ &= \frac{nr}{2} \cdot 2r(r-1)\sqrt{2} \\ &= nr^2(r-1)\sqrt{2}. \end{aligned}$$

Theorem 3.10. *Let G be an r-regular graph of order n, where $n \geq 2$. Then the reverse mass Sombor index of $r - regular$ is*

$$RMSO(r-regular) = \frac{nr}{\sqrt{2}}.$$

Proof. Let G be an r-regular graph of order n. Then, for every vertex $u \in V(G)$, $d(u) = r$
For each $uv \in E(G)$, the edge mass is defined by $w(uv) = d(u) + d(v) - 2$.
Since G is r-regular, $w(uv) = r + r - 2 = 2r(r-1)$. Every vertex is incident with r edges. Therefore, the mass degree of every vertex $u \in V(G)$ is

$$d^w(u) = r \cdot 2(r-1) = 2r(r-1).$$

Since all vertices have the same degree, $\Delta^w(r - regular) = 2r(r-1)$ By the definition of the reverse mass Sombor index,

$$\begin{aligned} RMSO(r-regular) &= \sum_{uv \in E(r-regular)} \sqrt{[2r(r-1) - 2r(r-1)+]^2 + [2r(r-1) - 2r(r-1)+1]^2} \\ &= \frac{nr}{2}\sqrt{2} \\ &= \frac{nr}{\sqrt{2}}. \end{aligned}$$

Theorem 3.11. *Let P_n be the path graph of order n, where $n \geq 5$. Then the mass Sombor index of P_n is*

$$MSO(P_n) = 2\sqrt{10} + 10 + 4(n-5)\sqrt{2}.$$

Proof. Let P_n be the path graph with vertex set

$$V(P_n) = \{u_1, u_2, \ldots, u_n\},$$

The two end vertices u_1 and u_n have degree 1, while $d(u_\ell) = 2$, $2 \leq \ell \leq n-1$.
For the edges u_1u_2 and $u_{n-1}u_n$, the mass of each edge is $w(u_1u_2) = w(u_{n-1}u_n) = 1 + 2 - 2 = 1$.
For the remaining edges $u_\ell u_{\ell+1}$, where $2 \leq \ell \leq n-2$, we have $w(u_\ell u_{\ell+1}) = 2 + 2 - 2 = 2$.
Therefore, the mass degrees of the vertices $d^w(u_1) = d^w(u_n) = 1$ and $d^w(u_2) = d^w(u_{n-1}) = 1 + 2 = 3$.
For every vertex u_ℓ, $3 \leq \ell \leq n-2, d^w(u_\ell) = 2 + 2 = 4$
Thus, the edge set of P_n can be classified according to the mass degrees of their end vertices as follows. By the definition of the mass Sombor index and the edge

TABLE 1. Edge classification according to the mass degrees of P_n.

$d^w(u), d^w(v), uv \in E(P_n)$	**Number of edges**
$(1, 3)$	2
$(3, 4)$	2
$(4, 4)$	$n-5$

classification as shown in Table 1, we obtain

$$\begin{aligned} MSO(P_n) &= 2\sqrt{1^2+3^2} + 2\sqrt{3^2+4^2} + (n-5)\sqrt{4^2+4^2} \\ &= 2\sqrt{10} + 10 + 4(n-5)\sqrt{2} \end{aligned}$$

Theorem 3.12. *Let P_n be the path graph of order n, where $n \geq 5$. Then the reverse mass Sombor index of P_n is*

$$RMSO(P_n) = 6\sqrt{5} + (n-5)\sqrt{2}.$$

Proof. From Theorem 3.9, the maximim mass degree of P_n is $\Delta^w(P_n) = 4$, using the edge classification given in Table 1, the reverse mass Sombor index of P_n is

$$\begin{aligned} RMSO(P_n) &= 2\sqrt{(4-1+1)^2+(4-3+1)^2} + 2\sqrt{(4-3+1)^2+(4-4+1)^2} \\ &\quad + (n-5)\sqrt{(4-4+1)^2+(4-4+1)^2} \\ &= 2\sqrt{4^2+2^2} + 2\sqrt{2^2+1^2} + (n-5)\sqrt{1+1} \\ &= 2\sqrt{20} + 2\sqrt{5} + (n-5)\sqrt{2} \\ &= 4\sqrt{5} + 2\sqrt{5} + (n-5)\sqrt{2} \\ &= 6\sqrt{5} + (n-5)\sqrt{2} \end{aligned}$$

4. Bounds for the mass Sombor index

In this section, we establish lower and upper bounds for the mass Sombor index in terms of the minimum and maximum mass degrees of a graph. Let G be a simple connected graph. The minimum and maximum mass degree of G are defined as:

$$\delta^w(G) = min\{d^w(u) : u \in V(G)\}$$

and

$$\Delta^w(G) = max\{d^w(u) : u \in V(G)\}$$

Theorem 4.1. *Let G be a simple connected graph with n vertices and m edges. Then*

$$\sqrt{2}m\delta^w(G) \leq MSO(G) \leq \sqrt{2}m\Delta^w(G).$$

Equality holds if and only if G is mass-regular graph.

Proof. For every edge $uv \in E(G)$, we have

$$\delta^w(G) \leq d^w(u),\ d^w(v) \leq \Delta^w(G).$$

Therefore,

$$\sqrt{2}\,\delta^w(G) \leq \sqrt{d^w(u)^2 + d^w(v)^2} \leq \sqrt{2}\,\Delta^w(G).$$

By the definition of the mass Sombor index, we obtain

$$\begin{aligned} MSO(G) &= \sum_{uv \in E(G)} \sqrt{d^w(u)^2 + d^w(v)^2} \\ &\leq \sum_{uv \in E(G)} \sqrt{\Delta^w(G)^2 + \Delta^w(G)^2} \\ &\leq m\Delta^w(G)\sqrt{2}. \end{aligned}$$

Similarly,

$$\begin{aligned} MSO(G) &= \sum_{uv \in E(G)} \sqrt{d^w(u)^2 + d^w(v)^2} \\ &\geq \sum_{uv \in E(G)} \sqrt{\delta^w(G)^2 + \delta^w(G)^2} \\ &\geq m\sqrt{2}\,\delta^w(G). \end{aligned}$$

Thus,

$$\sqrt{2}m\delta^w(G) \leq MSO(G) \leq \sqrt{2}m\Delta^w(G).$$

If G is mass-regular, then $\delta^w(G) = \Delta^w(G)$, and hence both inequalities become equal.

Conversely, suppose equality holds in either bound. Since G is connected, every vertex is incident with at least one edge. Equality in the corresponding edgewise inequality implies that every endpoint of every edge has the same mass degree. Hence,

$$\delta^w(G) = \Delta^w(G),$$

and therefore all vertices of G have the same mass degree. Thus, G is mass-regular. Therefore, equality holds if and only if G is mass-regular.

5. Chemical Applications: QSPR Analysis

Topological indices have been widely used as molecular descriptors in quantitative structure–property relationship (QSPR) studies to establish mathematical relationships between the structural characteristics of molecular graphs and their physicochemical properties. Such descriptors provide an efficient approach for predicting various physicochemical properties without requiring extensive experimental investigations. Motivated by these applications, the chemical applicability of the Mass Sombor index, denoted by $MSO(G)$, is investigated through QSPR analysis.

Correlation analysis between $MSO(G)$ and the physicochemical properties of Anti-Asthmatic drugs

To evaluate the predictive capability of the Mass Sombor index, a set of selected anti-asthmatic drugs is considered. In the present study, the Mass Sombor index $MSO(G)$ is treated as the independent variable, while the selected physicochemical properties are considered as dependent variables. The properties investigated are boiling point (BP), enthalpy of vaporization (E), flash point (FP), logP, molar volume (MV), and molar refractivity (MR).

For each anti-asthmatic drug, the corresponding value of $MSO(G)$ was computed from its molecular graph. The experimental values of the selected physicochemical properties were obtained from [1]. The calculated values of $MSO(G)$ along with the corresponding physicochemical properties are presented in Table 1. The obtained results were computed and verified using Maxima. Scatter plots illustrating the relationships between $MSO(G)$ and the selected physicochemical properties are presented in Figures 1–6. The corresponding correlation coefficients (R) and coefficients of determination (R^2) are summarized in Table 3.

The correlation analysis between the Mass Sombor Index and the selected physicochemical properties of anti-asthmatic drugs is presented in Table 3. The results indicate a strong positive correlation between the Mass Sombor Index and all the investigated properties. The highest correlation coefficient is observed for boiling point (BP), with $R = 0.9135$ and $R^2 = 0.8345$. Similarly, enthalpy of vaporization shows a strong correlation with $R = 0.9094$ and $R^2 = 0.8270$.

A strong positive correlation is also obtained for flash point (FP), with $R = 0.8819$ and $R^2 = 0.7777$, while molar refractivity (MR) exhibits a correlation coefficient of $R = 0.8907$ and a coefficient of determination of $R^2 = 0.7934$. The Mass Sombor Index also shows a strong correlation with logP, for which $R = 0.8626$ and $R^2 = 0.7441$ are obtained. The correlation with molar volume (MV) is comparatively lower but remains strong, with $R = 0.8367$ and $R^2 = 0.7000$.

TABLE 2. Mass Sombor index and physicochemical properties of Anti-Asthmatic drugs

Molecules	$MSO(G)$	BP	E	FP	$\log P$	MV	MR
Epinephrine	124.2	413.1	70.2	207.9	-0.63	142.7	49.3
Isoproterenol	145.4	417.5	70.7	179.7	0.25	176.2	58.6
Metaproterenol	143	417.5	70.7	179.7	0.13	176.1	58.6
Salbutamol	184.6	433.5	72.7	159.5	0.01	207.6	67.8
Terbutaline	174.9	419.2	70.9	165.3	0.48	192.3	63.2
Salmeterol	246.8	603	94.3	318.5	3.07	373.7	121.8
Formoterol	223.6	603.2	94.3	318.6	1.57	279.1	97.6
Vilanterol	254.3	646.7	100.2	344.9	2.97	387.5	128.7
Indacaterol	325.8	660.3	102.1	353.1	3.88	506.9	113.3
Olodaterol	323.1	649	100.5	346.3	1.17	308.o	105.1
Montelukast	489.8	750.5	114.8	407.7	7.80	460.8	173.7
Pranlukast	383.2	—	—	—	3.88	350.4	132.6
Zafirlukast	489.6	—	—	—	6.15	433.6	156.4
Ramatroban	358.1	654.7	101.3	349.7	4.09	289.7	107.5
Setipiprant	375.4	690.4	106.3	371.4	3.39	292.4	110.7
Fevipiprant	383.8	637.6	99	339.4	2.85	295.4	100.7
Abediterol	343.9	681.6	105	366	3.67	371.3	121.3
Bedoradrine	326.7	695.9	107	374.7	0.12	335.4	118.9
Toreforant	326.8	611.2	90.8	323.4	4.22	341.7	120.1

TABLE 3. Correlation coefficient (R) and coefficient of determination (R^2) between the mass Sombor index and Anti-Asthmatic drugs.

Property	R	R^2
Boiling point (BP)	0.9135	0.8345
Enthalpy of vaporization (E)	0.9094	0.827
Flash point (FP)	0.8819	0.7777
logP	0.8626	0.7441
Molar volume (MV)	0.8367	0.7
Molar refractivity (MR)	0.8907	0.7934

Overall, the obtained results demonstrate that the Mass Sombor Index has a strong positive relationship with the considered physicochemical properties of anti-asthmatic drugs. Among the investigated properties, boiling point exhibits the highest correlation, whereas molar volume shows the lowest correlation. These findings suggest that the Mass Sombor Index may be a useful molecular descriptor for quantitative structure–property relationship (QSPR) studies of anti-asthmatic drugs.

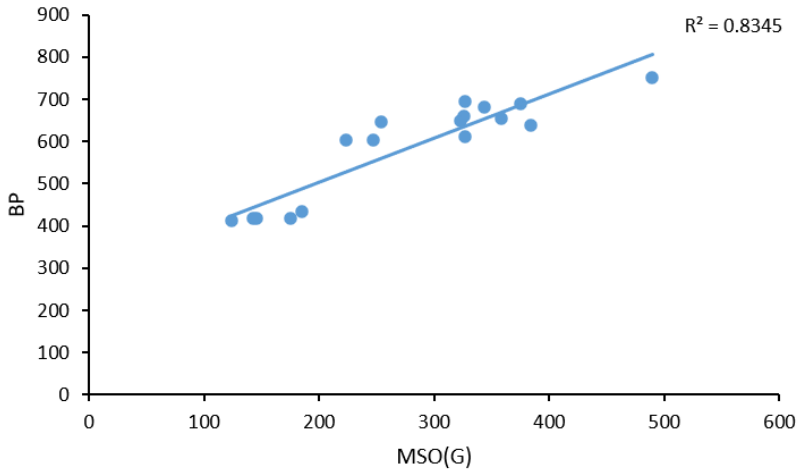


FIGURE 1

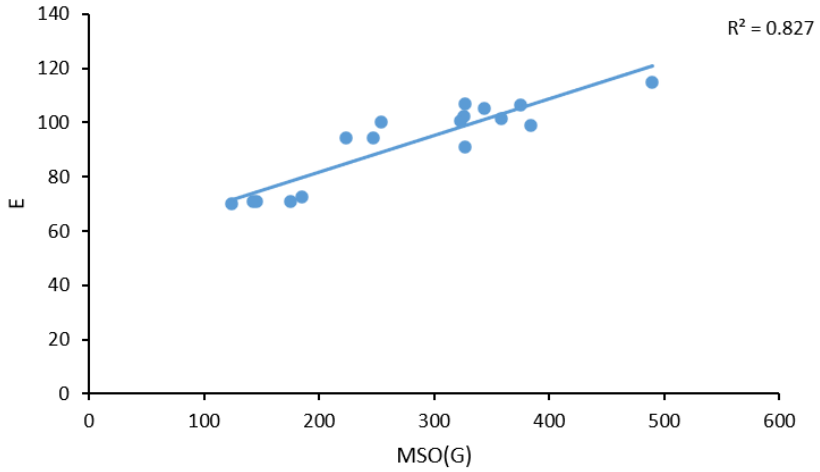


FIGURE 2

6. Conclusion

In this paper, we introduced the Mass Sombor index $MSO(G)$ and the Reverse Mass Sombor index $RMSO(G)$. Closed-form expressions were obtained for several standard graphs, including paths, cycles, complete graphs, wheel graphs, and regular graphs. Bounds for $MSO(G)$ were also established in terms of the minimum and maximum mass degrees.

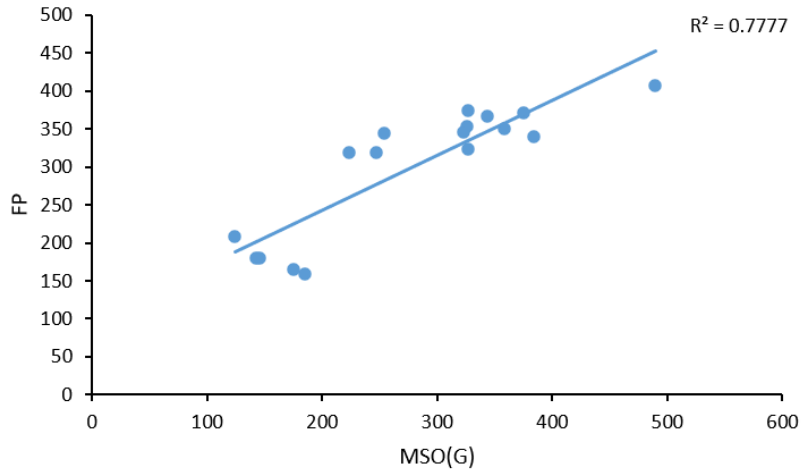


FIGURE 3

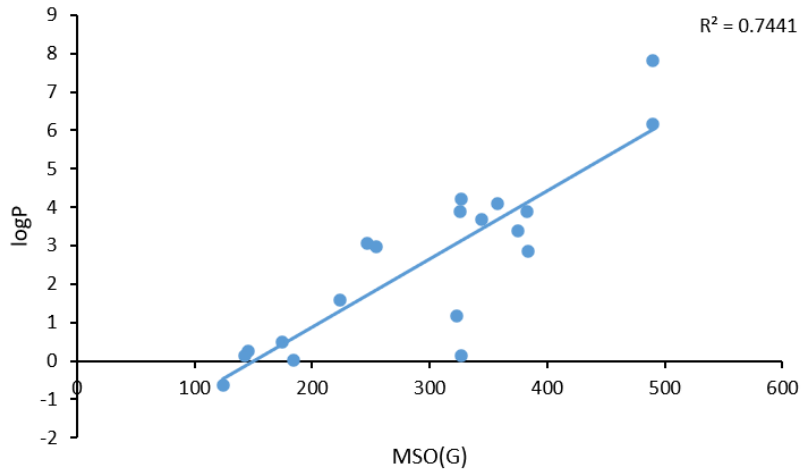


FIGURE 4

The chemical applicability of $MSO(G)$ was investigated using selected anti-asthmatic drugs. The correlation analysis showed strong positive relationships between $MSO(G)$ and the considered physicochemical properties. The highest correlation was observed with boiling point ($R = 0.9135$, $R^2 = 0.8345$), while molar volume showed the lowest correlation ($R = 0.8367$, $R^2 = 0.7000$).

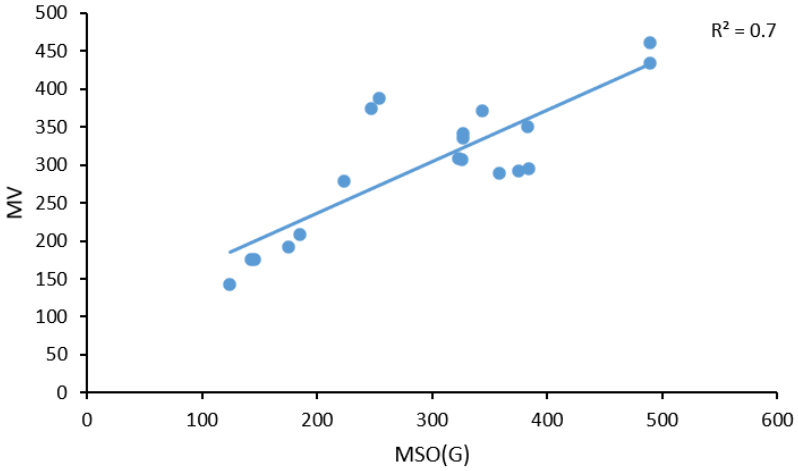


FIGURE 5

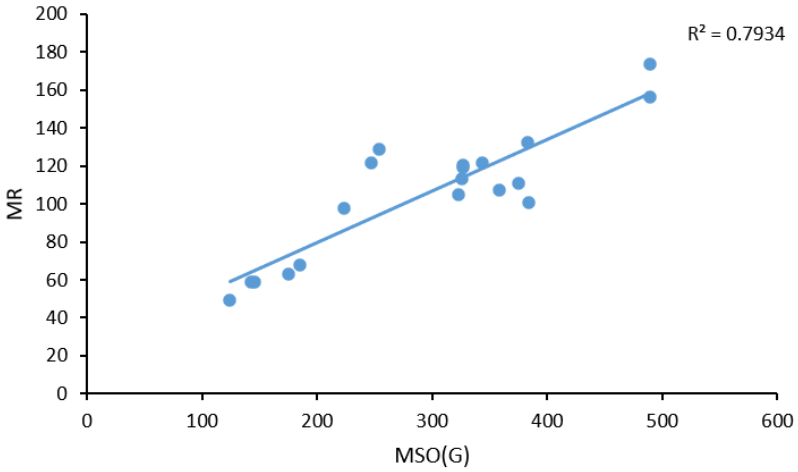


FIGURE 6

These results demonstrate that the Mass Sombor index is a promising molecular descriptor for QSPR studies and provide a basis for further investigation of mass-based Sombor-type indices.

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