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Multiplicative Version of Sombor Indices of Hyaluronic Acid-Curcumin, Methotrexate and Paclitaxel Conjugates

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Abstract: Numerous experiments have shown that the chemical properties of chemical compounds are closely related to their molecular structure. The molecular structure of corresponding drugs will be useful to precipitate the drug design and development process. Thus, the study of topological graph invariants of a drug structure helps to analyse the physio-chemical properties and biological properties of drugs. In this, paper the multiplicative sombor index, multiplicative reduced sombor index and multiplicative reduced modified sombor index of hyaluronic acid-curcumin, hyaluronic acid-methotrexate and hyaluronic acid-paclitaxel conjugates are determined by using vertex degree counting method. Finally, the comparative study of the indices will be discussed.

MSC: 05C05.

Keywords: Connectivity index, sombor index, hyaluronic acid-curcumin conjugates, hyaluronic acid-methotrexate conjugates.

1. Introduction

Chemical graph theory is the main branch of graph theory which deals with the mathematical modelling of chemical compound. In chemical graph every atom is expressed as a vertex and bonds are showed as an edge between the vertices. Topological graph index of a graph is the numerical value which can get from the chemical graph of a molecular. It indicates the some properties of the molecular graph. In recent decades many topological descriptors and its applications have been discussed [1–5]. Let K be a simple connected graph with vertex set is denoted by $V(K)$ and its edge set is denoted by $E(K)$ respectively. The degree of the vertex (a) is the number of adjacent vertices of a. It is denoted by $d_K(a)$.

The Sombor Index (SI) was proposed by Gutman [6], is defined as

$$SO(K) = \sum_{uv\in E(K)} \sqrt{d_K(a)^2 + d_K(b)^2}$$

Inspired by this, now we defined multiplicative SI of a graph K is

$$SOII(K) = \prod_{uv\in E(K)} \sqrt{d_K(a)^2 + d_K(b)^2} \tag{1}$$

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The Reduced Sombor Index (RSI) was introduced by Gutman [6] and it is defined as

$$RSO(K) = \sum_{uv \in E(K)} \sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2}$$

Now we define the multiplicative RSI of a graph is,

$$RSOII(K) = \prod_{uv \in E(K)} \sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2} \tag{2}$$

The Reduced Modified Sombor Index (RMSI) of a graph K was suggested by V. R. Kulli and I. Gutman [7], dined as

$$^{m}RSO(K) = \sum_{ab \in E(K)} \frac{1}{\sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2}}$$

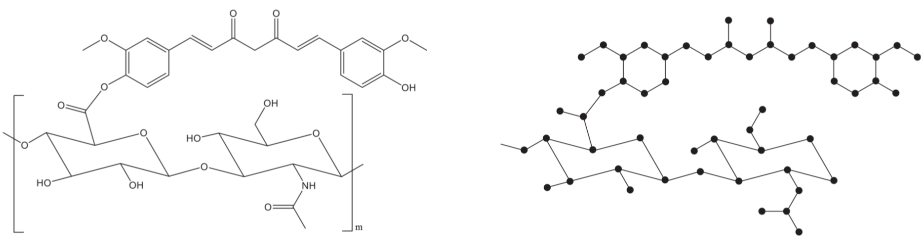
Now, we define the multiplicative RMSI of a graph K is defined as

$$^{m}RSOII(K) = \prod_{ab \in E(K)} \frac{1}{\sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2}} \tag{3}$$

In this article, the multiplicative SI, multiplicative RSI, multiplicative RMSI of Hyaluronic Acid-Curcumin (HA-CC), Hyaluronic Acid-Methotrexate (HA-MT), and Hyaluronic Acid-Paclitaxel will be calculated.

2. Results for HA-CC

In this section, the graph connectivity index of HA-CC conjugate will be computed by using Vertex-degree counting based. The chemical graph of HA-CC is showed in Figure 1.



(a) Chemical Structure of HA-CC Conjugate (b) Molecular Graph of HA-CC Conjugate: $m = 1$

Figure 1.

Lemma 2.1. *Let HC_m be the chemical graph of HA-CC conjugates with m units, then the following values can be found by edge partitioning method.*

Table 1.

$E_1 = (1,2)$	$E_2 = (1,3)$	$E_3 = (2,2)$	$E_4 = (3,3)$	$E_5 = (2,3)$	$\|V\|$	$\|E\|$
$3m+1$	$9m$	$4m+1$	$11m-1$	$29m-1$	$52m+1$	$56m$

Theorem 2.2. *Let HC_m denote the chemical graph of HA-CC conjugates, then*

(1). $SOII(HC_m) = 2^{16m+1} \times 3^{11m-1} \times 5^{6m+\frac{1}{2}} \times 13^{\frac{29m}{2}-\frac{1}{2}}$.

(2). $RSOII(HC_m) = 2^{\frac{55m}{2}-1} \times 5^{\frac{29m}{2}-\frac{1}{2}}$.

(3). ${}^{m}RSOII(HC_m) = 2^{1-\frac{55m}{2}} \times 5^{\frac{29m}{2}-\frac{1}{2}}$.

Proof. Using the definition of graph connectivity indices and the Table 1 from Lemma 2.1, we have

(1).
$$SOII(K) = \prod_{ab\in E(K)} \sqrt{d_K(a)^2 + d_K(b)^2}$$

$$\begin{aligned}
SOII(HC_m) &= \prod_{ab\in E(HC_m)} \sqrt{d_{HC_m}(a)^2 + d_{HC_m}(b)^2} \\
&= \prod_{ab\in E_1} \sqrt{1^2+2^2} \times \prod_{ab\in E_2} \sqrt{1^2+3^2} \times \prod_{ab\in E_3} \sqrt{2^2+2^2} \times \prod_{ab\in E_4} \sqrt{3^2+3^2} \times \prod_{ab\in E_5} \sqrt{2^2+3^2} \\
&= (\sqrt{5})^{3m+1} \times (\sqrt{10})^{9m} \times (\sqrt{8})^{4m+1} \times (\sqrt{18})^{11m-1} \times (\sqrt{13})^{29m-1} \\
&= 2^{16m+1} \times 3^{11m-1} \times 5^{6m+\frac{1}{2}} \times 13^{\frac{29m}{2}-\frac{1}{2}}
\end{aligned}$$

(2).
$$RSOII(K) = \prod_{ab\in E(K)} \sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2}$$

$$\begin{aligned}
RSOII(HC_m) &= \prod_{ab\in E(HC_m)} \sqrt{(d_{HC_m}(a)-1)^2 + (d_{HC_m}(b)-1)^2} \\
&= \prod_{ab\in E_1} \sqrt{(1-1)^2+(2-1)^2} \times \prod_{ab\in E_2} \sqrt{(1-1)^2+(3-1)^2} \times \prod_{ab\in E_3} \sqrt{(2-1)^2+(2-1)^2} \\
&\times \prod_{ab\in E_4} \sqrt{(3-1)^2+(3-1)^2} \times \prod_{ab\in E_5} \sqrt{(2-1)^2+(3-1)^2} \\
&= (1)^{3m+1} \times 2^{9m} \times (\sqrt{2})^{4m+1} \times (\sqrt{8})^{11m-1} \times (\sqrt{5})^{29m-1} \\
&= 2^{\frac{55m}{2}-1} \times 5^{\frac{29m}{2}-\frac{1}{2}}
\end{aligned}$$

(3).
$${}^{m}RSOII(K) = \prod_{ab\in E(K)} \frac{1}{\sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2}}$$

$$\begin{aligned}
{}^{m}RSOII(HC_m) &= \prod_{ab\in E(HC_m)} \frac{1}{\sqrt{(d_{HC_m}(a)-1)^2 + (d_{HC_m}(b)-1)^2}} \\
&= \prod_{ab\in E_1} \frac{1}{\sqrt{(1-1)^2+(2-1)^2}} \times \prod_{ab\in E_2} \frac{1}{\sqrt{(1-1)^2+(3-1)^2}} \times \prod_{ab\in E_3} \frac{1}{\sqrt{(2-1)^2+(2-1)^2}} \\
&\times \prod_{ab\in E_4} \frac{1}{\sqrt{(3-1)^2+(3-1)^2}} \times \prod_{ab\in E_5} \frac{1}{\sqrt{(2-1)^2+(3-1)^2}} \\
&= \left(\frac{1}{\sqrt{0+1}}\right)^{3m+1} \times \left(\frac{1}{\sqrt{4}}\right)^{9m} \times \left(\frac{1}{\sqrt{1+1}}\right)^{4m+1} \times \left(\frac{1}{\sqrt{4+4}}\right)^{11m-1} \times \left(\frac{1}{\sqrt{1+4}}\right)^{29m-1} \\
&= 1 \times \left(\frac{1}{2}\right)^{9m} \times \left(\frac{1}{\sqrt{2}}\right)^{4m+1} \times \left(\frac{1}{\sqrt{8}}\right)^{11m-1} \times \left(\frac{1}{\sqrt{5}}\right)^{29m-1} \\
&= 2^{1-\frac{55m}{2}} \times 5^{\frac{1}{2}-\frac{29m}{2}}
\end{aligned}$$

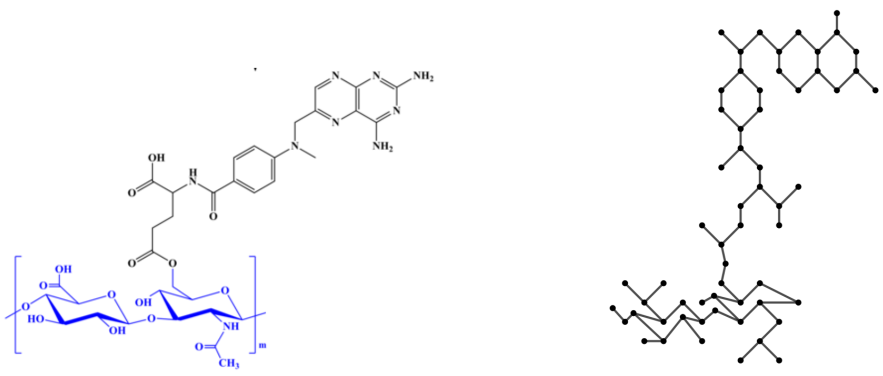
HC_m	$SOII(HC_m)$	$RSOII(HC_m)$	${}^{m}RSOII(HC_m)$
$m=1$	$1.0647176021 \times 10^{30}$	$5.7926187514 \times 10^{17}$	$1.72633491500 \times 10^{-18}$
$m=2$	$2.741869286 \times 10^{60}$	$1.50059981796 \times 10^{36}$	$6.66400187462 \times 10^{-37}$

Table 2. **Comparison of the multiplicative SI, multiplicative RSI, multiplicative RMSI HC_m of the molecular structure**

□

3. Results for HA-MT

In this section, the graph connectivity index of HA-MT conjugate will be computed by using vertex-degree counting based. The chemical graph of HA-MT is showed in Figure 2.



(a) Chemical Structure of HA-MT Conjugate

(b) Molecular Graph of HA-MT Conjugate: $m = 1$

Figure 2.

Lemma 3.1. *Let HC_m be the chemical graph of HA-MT conjugates with m units, then the following results will be holds.*

Table 3.

$E_1 = (1,2)$	$E_2 = (1,3)$	$E_3 = (2,2)$	$E_4 = (3,3)$	$E_5 = (2,3)$	$\|V\|$	$\|E\|$
1	$14m$	$5m+1$	$14m-1$	$30m-1$	$58m+1$	$63m$

Theorem 3.2. *Let HM_m denote the chemical graph of HA-MT conjugates, then*

(1). $SOII(HM_m) = 2^{\frac{43m}{2}+1} \times 3^{14m-1} \times 5^{7m+\frac{1}{2}} \times 13^{15m-\frac{1}{2}}$.

(2). $RSOII(HM_m) = 2^{\frac{75m}{2}-1} \times 5^{15m-\frac{1}{2}}$.

(3). ${}^{m}RSOII(HM_m) = 2^{1-\frac{75m}{2}} \times 5^{\frac{1}{2}-15m}$.

Proof. Using the definition of graph connectivity indices and the Table 6 from Lemma 3.1, we have

(1).
$$SOII(K) = \prod_{ab\in E(K)} \sqrt{d_K(a)^2 + d_K(b)^2}$$

$$\begin{aligned}
SOII(HM_m) &= \prod_{ab\in E(HM_m)} \sqrt{d_{HM_m}(a)^2 + d_{HM_m}(b)^2} \\
&= \prod_{ab\in E_1} \sqrt{1^2+2^2} \times \prod_{ab\in E_2} \sqrt{1^2+3^2} \times \prod_{ab\in E_3} \sqrt{2^2+2^2} \times \prod_{ab\in E_4} \sqrt{3^2+3^2} \times \prod_{ab\in E_5} \sqrt{2^2+3^2} \\
&= (\sqrt{5})^1 \times (\sqrt{10})^{14m} \times (\sqrt{8})^{5m+1} \times (\sqrt{18})^{14m-1} \times (\sqrt{13})^{30m-1} \\
&= 2^{\frac{43m}{2}+1} \times 3^{14m-1} \times 5^{7m+\frac{1}{2}} \times 13^{15m-\frac{1}{2}}
\end{aligned}$$

(2). $$RSOII(K) = \prod_{ab\in E(K)} \sqrt{(d_K(a)-1)^2+(d_K(b)-1)^2}$$

$$\begin{aligned}
RSOII(HM_m) &= \prod_{ab\in E(HM_m)} \sqrt{(d_{HM_m}(a)-1)^2+(d_{HM_m}(b)-1)^2}\\
&= \prod_{ab\in E_1}\sqrt{(1-1)^2+(2-1)^2}\times\prod_{ab\in E_2}\sqrt{(1-1)^2+(3-1)^2}\times\prod_{ab\in E_3}\sqrt{(2-1)^2+(2-1)^2}\\
&\quad\times\prod_{ab\in E_4}\sqrt{(3-1)^2+(3-1)^2}\times\prod_{ab\in E_5}\sqrt{(2-1)^2+(3-1)^2}\\
&= (1)^1\times 2^{14m}\times(\sqrt{2})^{5m+1}\times(\sqrt{8})^{14m-1}\times(\sqrt{5})^{30m-1}\\
&= 2^{\frac{75m}{2}-1}\times 5^{15m-\frac{1}{2}}
\end{aligned}$$

(3). $$^{m}RSOII(K) = \prod_{ab\in E(K)} \frac{1}{\sqrt{(d_K(a)-1)^2+(d_K(b)-1)^2}}$$

$$\begin{aligned}
^{m}RSOII(HM_m) &= \prod_{ab\in E(HM_m)} \frac{1}{\sqrt{(d_{HM_m}(a)-1)^2+(d_{HM_m}(b)-1)^2}}\\
&= \prod_{ab\in E_1}\frac{1}{\sqrt{(1-1)^2+(2-1)^2}}\times\prod_{ab\in E_2}\frac{1}{\sqrt{(1-1)^2+(3-1)^2}}\times\prod_{ab\in E_3}\frac{1}{\sqrt{(2-1)^2+(2-1)^2}}\\
&\quad\times\prod_{ab\in E_4}\frac{1}{\sqrt{(3-1)^2+(3-1)^2}}\times\prod_{ab\in E_5}\frac{1}{\sqrt{(2-1)^2+(3-1)^2}}\\
&= \left(\frac{1}{\sqrt{0+1}}\right)^{3m+1}\times\left(\frac{1}{\sqrt{4}}\right)^{14m}\times\left(\frac{1}{\sqrt{1+1}}\right)^{5m+1}\times\left(\frac{1}{\sqrt{4+4}}\right)^{14m-1}\times\left(\frac{1}{\sqrt{1+4}}\right)^{30m-1}\\
&= 2^{1-\frac{75m}{2}}\times 5^{\frac{1}{2}-15m}
\end{aligned}$$

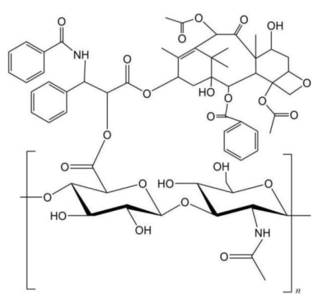
HM_m	$SOII(HM_m)$	$RSOII(HM_m)$	$^{m}RSOII(HM_m)$
$m=1$	$2.3453348383\times10^{34}$	$1.3263553839\times10^{21}$	$7.5394574646\times10^{-22}$
$m=2$	$1.3304165617\times10^{39}$	$7.8674647736\times10^{42}$	$1.2710574864\times10^{-43}$

Table 4. **Comparison of the multiplicative SI, multiplicative RSI, multiplicative RMSI HC_m of the molecular structure**

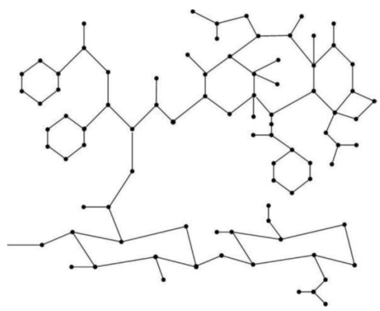
□

4. Results for HA-PT

In this section, the graph connectivity index of HA-PT conjugates are computed by using vertex-degree counting based. The chemical graph of HA-PT is showed in Figure 3.



(a) Chemical Structure of HA-PT Conjugate



(b) Molecular Graph of HA-PT Conjugate: $m = 1$

Figure 3.

Lemma 4.1. *Let HP_m be the chemical graph of HA-PT conjugates with m units, then the following values can be found by edge partitioning method.*

Table 5.

$E_1 = (1,2)$	$2m$	$E_7 = (2,4)$	$3m$
$E_2 = (1,3)$	$16m$	$E_8 = (3,4)$	$7m$
$E_3 = (2,2)$	$13m+1$	$E_9 = (4,4)$	$2m$
$E_4 = (3,3)$	$19m-1$	$\|V\|$	$87m$
$E_5 = (2,3)$	$33m-1$	$\|E\|$	$96m$
$E_6 = (1,4)$	$4m$		

Theorem 4.2. *Let HP_m denote the chemical graph of HA-PT conjugates, then*

(1). $SOII(HP_m) = 2^{45m+1} \times 3^{19m-1} \times 5^{\frac{35m}{2}} \times 13^{\frac{33m-1}{2}} \times 17^{2m}$.

(2). $RSOII(HP_m) = 2^{\frac{107m}{2}-1} \times 3^{6m} \times 5^{18m-\frac{1}{2}} \times 13^{\frac{7m}{2}}$.

(3). ${}^{m}RSOII(HP_m) = 2^{1-\frac{107m}{2}} \times 3^{-6m} \times 5^{\frac{1}{2}-18m} \times 13^{\frac{-7m}{2}}$.

Proof. Using the definition of graph connectivity indices and the Table 5 from Lemma 4.1, we have

(1).
$$SOII(K) = \prod_{ab\in E(K)} \sqrt{d_K(a)^2 + d_K(b)^2}$$

$$SOII(HM_m) = \prod_{ab\in E(HP_m)} \sqrt{d_{HP_m}(a)^2 + d_{HP_m}(b)^2}$$

$$= \prod_{ab\in E_1} \sqrt{1^2+2^2} \times \prod_{ab\in E_2} \sqrt{1^2+3^2} \times \prod_{ab\in E_3} \sqrt{2^2+2^2} \times \prod_{ab\in E_4} \sqrt{3^2+3^2} \times \prod_{ab\in E_5} \sqrt{2^2+3^2}$$

$$\times \prod_{ab\in E_6} \sqrt{1^2+4^2} \times \prod_{ab\in E_7} \sqrt{2^2+4^2} \times \prod_{ab\in E_8} \sqrt{3^2+4^2} \times \prod_{ab\in E_9} \sqrt{4^2+4^2}$$

$$= (\sqrt{5})^{2m} \times (\sqrt{10})^{16m} \times (\sqrt{8})^{13m+1} \times (\sqrt{18})^{19m-1} \times (\sqrt{13})^{33m-1} \times (\sqrt{17})^{4m} \times (\sqrt{20})^{3m}$$

$$\times (\sqrt{5})^{7m} \times (\sqrt{32})^{2m}$$

$$= 2^{45m+1} \times 3^{19m-1} \times 5^{\frac{35m}{2}} \times 13^{\frac{33m-1}{2}} \times 17^{2m}$$

(2).
$$RSOII(K) = \prod_{ab\in E(K)} \sqrt{(d_K(a)-1)^2 + (d_K(b)-1)^2}$$

$$RSOII(HP_m) = \prod_{ab\in E(HP_m)} \sqrt{(d_{HP_m}(a)-1)^2 + (d_{HP_m}(b)-1)^2}$$

$$= \prod_{ab\in E_1} \sqrt{(1-1)^2+(2-1)^2} \times \prod_{ab\in E_2} \sqrt{(1-1)^2+(3-1)^2} \times \prod_{ab\in E_3} \sqrt{(2-1)^2+(2-1)^2}$$

$$\times \prod_{ab\in E_4} \sqrt{(3-1)^2+(3-1)^2} \times \prod_{ab\in E_5} \sqrt{(2-1)^2+(3-1)^2} \times \prod_{ab\in E_6} \sqrt{(1-1)^2+(4-1)^2}$$

$$\times \prod_{ab\in E_7} \sqrt{(2-1)^2+(4-1)^2} \times \prod_{ab\in E_8} \sqrt{(3-1)^2+(4-1)^2} \times \prod_{ab\in E_9} \sqrt{(4-1)^2+(4-1)^2}$$

$$= (1)^{2m} \times 2^{16m} \times (\sqrt{2})^{13m+1} \times (\sqrt{8})^{19m-1} \times (\sqrt{5})^{33m-1} \times (\sqrt{3})^{4m} \times (\sqrt{10})^{3m}$$

$$\times (\sqrt{13})^{7m} \times (\sqrt{18})^{2m}$$

$$= 2^{\frac{107m}{2}-1} \times 3^{6m} \times 5^{18m-\frac{1}{2}} \times 13^{\frac{7m}{2}}$$

(3). $${}^{m}RSOII(K) = \prod_{ab\in E(K)} \frac{1}{\sqrt{(d_K(a)-1)^2+(d_K(b)-1)^2}}$$

$$\begin{aligned}
{}^{m}RSOII(HP_m) &= \prod_{ab\in E(HP_m)} \frac{1}{\sqrt{(d_{HP_m}(a)-1)^2+(d_{HP_m}(b)-1)^2}} \\
&= \prod_{ab\in E_1} \frac{1}{\sqrt{(1-1)^2+(2-1)^2}} \times \prod_{ab\in E_2} \frac{1}{\sqrt{(1-1)^2+(3-1)^2}} \times \prod_{ab\in E_3} \frac{1}{\sqrt{(2-1)^2+(2-1)^2}} \\
&\times \prod_{ab\in E_4} \frac{1}{\sqrt{(3-1)^2+(3-1)^2}} \times \prod_{ab\in E_5} \frac{1}{\sqrt{(2-1)^2+(3-1)^2}} \times \prod_{ab\in E_6} \frac{1}{\sqrt{(1-1)^2+(4-1)^2}} \\
&\times \prod_{ab\in E_7} \frac{1}{\sqrt{(2-1)^2+(4-1)^2}} \times \prod_{ab\in E_8} \frac{1}{\sqrt{(3-1)^2+(4-1)^2}} \times \prod_{ab\in E_9} \frac{1}{\sqrt{(4-1)^2+(4-1)^2}} \\
&= 1^{2m} \times \left(\frac{1}{\sqrt{4}}\right)^{16m} \times \left(\frac{1}{\sqrt{2}}\right)^{13m+1} \times \left(\frac{1}{\sqrt{8}}\right)^{19m-1} \times \left(\frac{1}{\sqrt{5}}\right)^{33m-1} \\
&\times \left(\frac{1}{\sqrt{9}}\right)^{4m} \times \left(\frac{1}{\sqrt{10}}\right)^{3m} \times \left(\frac{1}{\sqrt{13}}\right)^{7m} \times \left(\frac{1}{\sqrt{18}}\right)^{2m} \\
&= 2^{1-\frac{107m}{2}} \times 3^{-6m} \times 5^{\frac{1}{2}-18m} \times 13^{\frac{-7m}{2}}
\end{aligned}$$

Table 6. **Comparison of the multiplicative SI, multiplicative RSI, multiplicative RMSI HP_m of the molecular structure**

HP_m	$SOII(HP_m)$	$RSOII(HP_m)$	${}^{m}RSOII(HP_m)$
$m=1$	$8.943941316694 \times 10^{54}$	$6.2744997976 \times 10^{34}$	$1.593752541633 \times 10^{-35}$
$m=2$	$4.3263416970 \times 10^{110}$	$1.7606507542 \times 10^{70}$	$5.6797181246 \times 10^{-71}$

□

5. Conclusion

In this article, we obtained SI, RSI, MRSI of Hyaluronic Acid-Curcumin conjugates, Hyaluronic Acid-Methotreate and Hyaluronic Acid-Paclitaxel conjugates. Additionally, comparison of the indices found easily as the values of m. Since SI and RSI are in increasing order and MRSI is in decreasing order. This study leads to develop the drug design in medical field.

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