Letters in Applied NanoBioScience
Open-Access Journal (ISSN: 2284-6808)

Article
Volume 12, Issue 4, 2023, 143
https://doi.org/10.33263/LIANBS124.143

A Study of Hyaluronic Acid-Anticancer Drug Conjugates Via New *ve*-Degree Topological Indices

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Received: 28.08.2022; Accepted: 7.10.2022; Published: 17.11.2022

Abstract: The molecular structure of a compound contains all the information that would help determine its chemical, biological, and physical properties. One can assess these properties with the help of a theoretical descriptor tool known as topological indices. Recently, the ve-degree version of the Sombor index (SO_{ve}), Nirmala index(N_{ve}), and Misbalance prodeg index(MPI_{ve}) has been defined. A topological index is a unique numerical value attached to the structural graph of a molecule and is helpful in predicting the molecule's certain chemical/physical properties. In this paper, we compute SO_{ve}, N_{ve}, and MPI_{ve} of hyaluronic acid-curcumin/paclitaxel conjugates, known for their potential anti-inflammatory, antioxidant, and anticancer properties. These results are may helpful from chemical science and pharmaceutical points of view.

Keywords: hyaluronic acid-curcumin/paclitaxel conjugates; vertex-edge degree; topological indices.

1. Introduction

Pharmaceutical and chemical technologies are growing in exponential form. Due to this, a large number of new drugs are produced every year. An extensive quantity of work is required to establish drug pharmacological, chemical, and biological characteristics, which help develop medicines. Chemical experiments are required to determine these newly produced compounds and drugs' pharmacological, chemical, and biological properties. This will eventually increase the workload of pharmaceutical and chemical researchers. If these properties of the drugs can be predicted without any lab, it will reduce the workload of researchers. This can be done by analyzing the molecular structure of a relevant drug using a well-recognized tool of chemical graph theory known as the topological index. The numerical values associated with the chemical constitution are known as Topological indices, which are used to correlate chemical structure with numerous characteristics such as chemical reactivity, pharmacological activity, and physical properties. Topological indices have been used to explain and advance the statistical features of drugs. Topological indices play a crucial role in the quantitative structure-property relationship ($QSAR$) and the quantitative structure-activity relationship ($QSPR$) in predicting different physicochemical properties and bioactivity that contribute to the finding of new drugs [1,2]. Graph theory played a significant role in molecular chemistry, robotics, physics, networks, computer science, statistics, biological activities, and data science. A topological index is a unique number mathematically derived from the graph structure. In theoretical chemistry, many such topological indices have been considered and have more applications in a quantitative structure-property relationship ($QSPR$) and

quantitative structure-activity relationship $(QSAR)$ [3- 5]. The vertex-edge topological indices are gaining more interest in applied sciences [6- 12]. Let $G = (V, E)$ be the structure of the drugs, where each vertex indicates an atom and each edge represents a chemical bond between the atoms. The number of edges that are incident with the vertex u is known as the degree of the vertex u and is denoted by $d(u)$. The set $N(u) = \{u \in V(G) : uw \in E(G)\}$ and $N[u] = N(u) \cup \{u\}$iscalled as an open and closed neighborhood of the vertex u. The number of different edges that are incident to any vertex from $N[u]$, denoted by $d_{ve}(u)$ and called ve-degree [7]. Recently, new topological indices have been defined; the Sombor index $(SO(G))$[13], Nirmala index $N(G)$[14], and Misbalance prodeg index $MPI(G)$[15]. Some properties of the Sombor and Nirmala indices have been studied in [15,16]. The application of the Sombor index is studied and found in [17-20]. The ve-degree Sombor index SO_{ve} [21], the ve-degree Nirmala index (N_{ve}) [22], and the ve-degree Misbalance prodeg index MPI_{ve} [22] are defined as$SO_{ve} = \sum_{uw \in E} \sqrt{d_{ve}(u)^2 + d_{ve}(w)^2}$, $N_{ve} = \sum_{uw \in E} \sqrt{d_{ve}(u) + d_{ve}(w)}$, and $MPI_{ve} = \sum_{uw \in E} \sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)}$ respectively.

2. Materials and Methods

2.1. Hyaluronic acid-curcumin conjugate.

Let G_n be the molecular graph of hyaluronic acid-curcumin conjugates (HAC) with the linear iteration n units. For iterations 1 and 3, units are shown in Figure 1. By the graph structure analysis, we found the edge set of HAC can is divided into 17 edge groups based on the ve-degree of its end vertices which can be seen in Table 1.

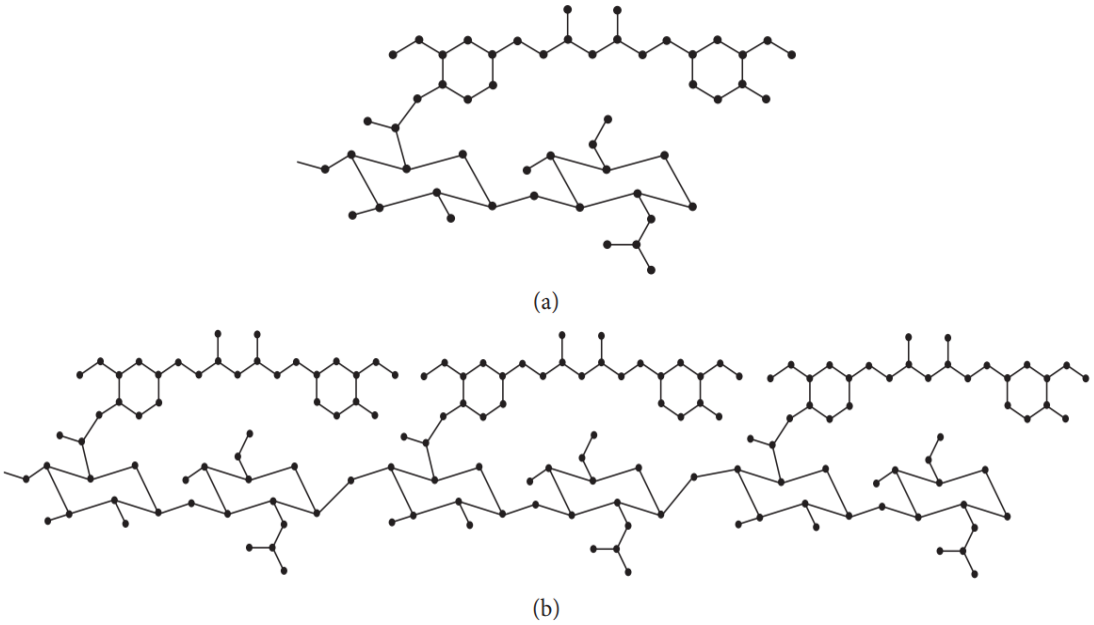

Figure 1. Corresponding molecular graph of hyaluronic acid-curcumin conjugates HAC (a.) for $n = 1$ and (b.) for $n = 3$.

Table 1. Edge partition of HAC, based on ve-degree.

Frequency of edges	$(d_{ve}(u), d_{ve}(w))$
$3n + 1$	(2,4)
$2n$	(3,4)
$2n$	(3,5)
$2n$	(3,6)
$3n$	(3,7)

Frequency of edges	$(d_{ve}(u), d_{ve}(w))$
$6n+1$	(5,5)
1	(4,8)
$9n-2$	(6,7)
$5n-2$	(6,8)
$3n$	(4,7)
$n+2$	(5,7)
n	(4,6)
$3n$	(6,6)
$7n$	(5,6)
$2n-1$	(8,8)
$3n$	(7,8)
$4n$	(7,7)

2.2. Hyaluronic acid-paclitaxel conjugate.

Let HAP be the molecular graph of Hyaluronic Acid-Paclitaxel Conjugates with the linear iteration n units. The corresponding molecular graph of HAP with iterations 1 and 3 is found in Figure 2. The edge partition of HAP can be found in Table 2.

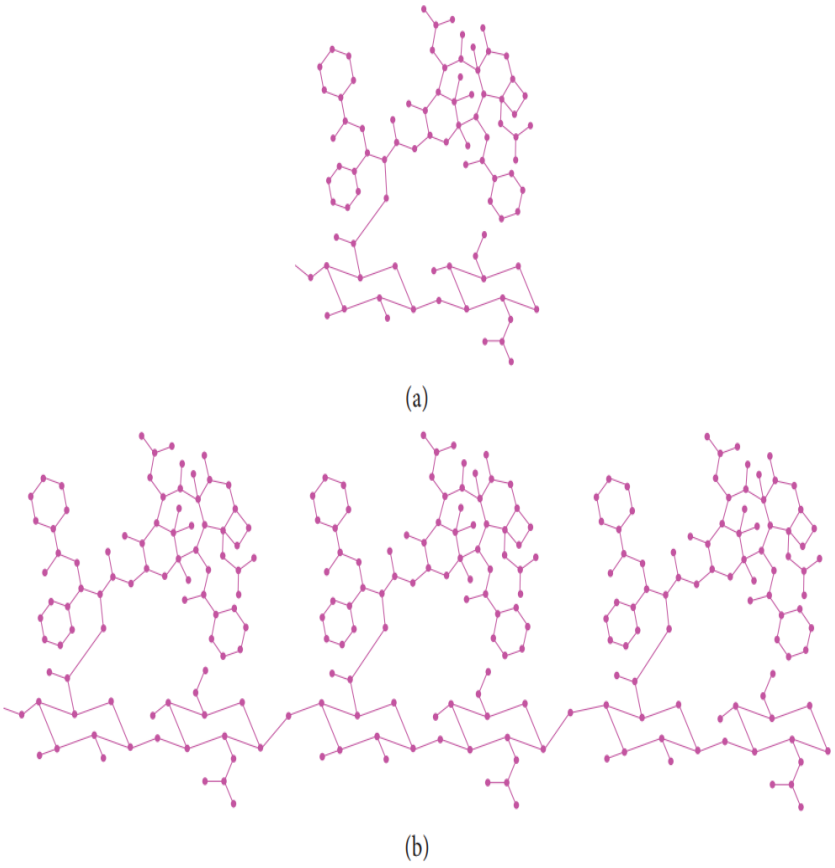

Figure 2. Corresponding molecular graph of hyaluronic acid-paclitaxel conjugates HAP (a.) for $n = 1$ and (b.) for $n = 3$.

Table 2. Edge partition of HAC, based on ve-degree.

Frequency of edges	$(\mathbf{d_{ve}(u)}, \mathbf{d_{ve}(w)})$	Frequency of edges	$(\mathbf{d_{ve}(u)}, \mathbf{d_{ve}(w)})$
$n+1$	(2,4)	n	(5,8)
$6n$	(3,4)	4n	(6,6)
$4n$	(3,6)	$9n-2$	(6,7)
$5n$	(3,7)	$10n-2$	(6,8)
n	(3,8)	n	(6,9)
$6n$	(4,4)	n	(6,10)

Frequency of edges	$(\mathbf{d_{ve}(u)}, \mathbf{d_{ve}(w)})$	Frequency of edges	$(\mathbf{d_{ve}(u)}, \mathbf{d_{ve}(w)})$
$6n$	(4,5)	5n	(7,7)
$2n$	(4,6)	4n	(7,8)
$2n$	(4,7)	4n	(7,10)
1	(4,8)	$4n-1$	(8,8)
$2n$	(4,9)	3n	(8,10)
$2n$	(4,10)	3n	(9,10)
1	(5,5)	n	(9,11)
n	(5,6)	2n	(10,11)
$6n+2$	(5,7)	–	–

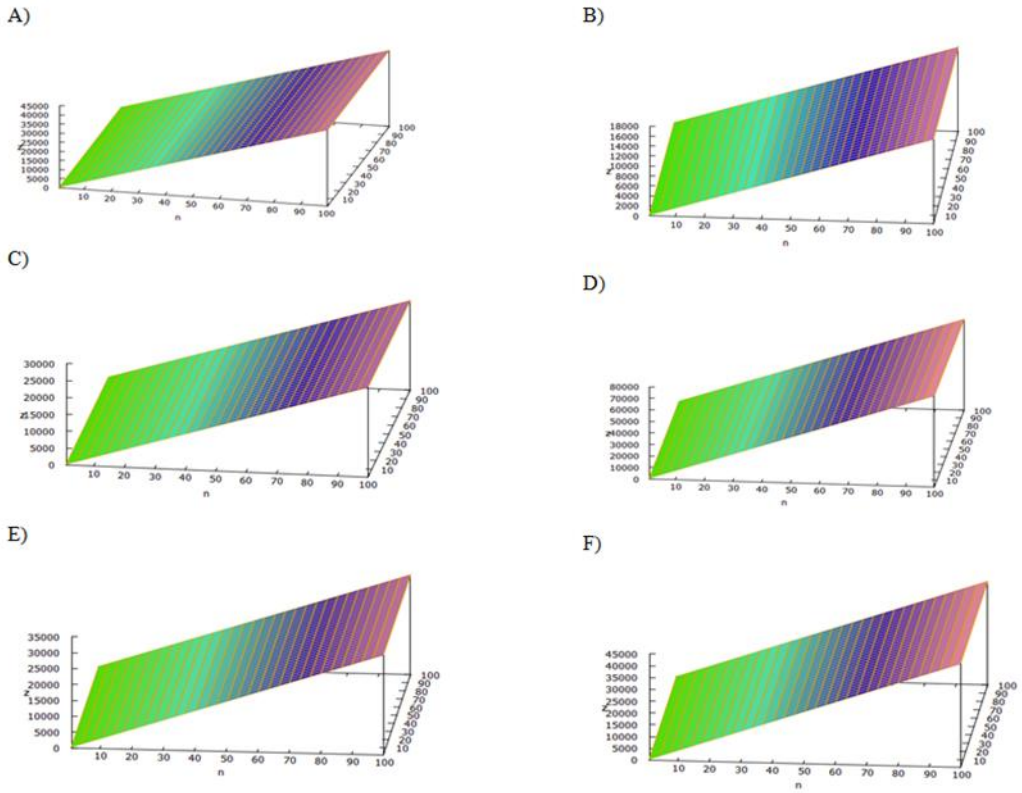

Figure 3. The 3-D graphical comparison of SO_{ve}, N_{ve}, and MPI_{ve} for HAC (A, B, and C), and (b.) for HAP(D, E, F) respectively.

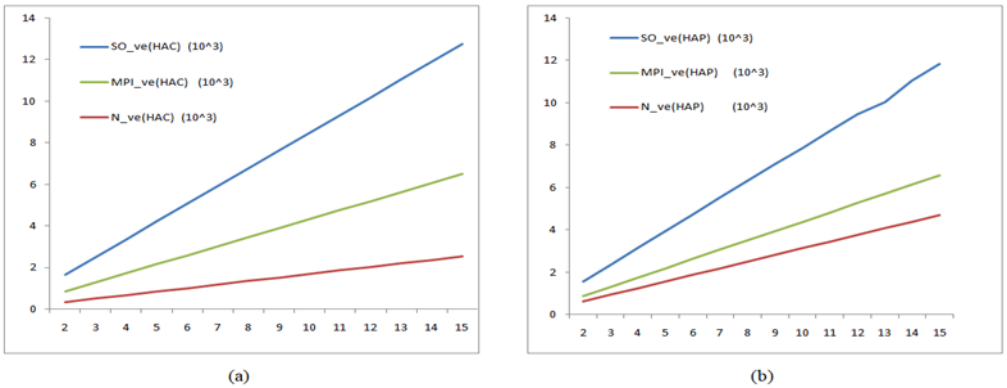

Figure 4. The graphical line comparison of $\boldsymbol{SO_{ve}}$, $\boldsymbol{N_{ve}}$, and $\boldsymbol{MPI_{ve}}$(a.) for HAC and (b.) for HAP.

3. Results and Discussion

3.1. Result for hyaluronic acid-curcumin conjugate.

Theorem 3.1.1. Let HAC be the HA-curcumin conjugate. Then,

i. $SO_{ve}(HAC) = (3n+1)\sqrt{20} + (9n-2)\sqrt{84} + (5n-2)10 + (n+2)\sqrt{74} + (2n-1)\sqrt{128} + n[10 + 2\sqrt{34} + 2\sqrt{45} + 3\sqrt{58} + 3\sqrt{65} + \sqrt{52} + 3\sqrt{72} + 7\sqrt{61} + 3\sqrt{113} + 4\sqrt{98}]$,

ii. $N_{ve}(HAC) = (3n+1)\sqrt{6} + (9n-2)\sqrt{13} + (5n-2)\sqrt{14} + (n+2)\sqrt{12} + 4(2n-1) + n[2\sqrt{7} + 2\sqrt{8} + 3\sqrt{10} + 3\sqrt{11} + \sqrt{10} + 6\sqrt{3} + 7\sqrt{11} + 3\sqrt{15} + 4\sqrt{14} + 6]$,

iii. $MPI_{ve}(HAC) = (3n+1)(\sqrt{2}+2) + (6n+1)(2\sqrt{5}) + (9n-2)(\sqrt{6}+\sqrt{7}) + (n+2)(\sqrt{5}+\sqrt{7}) + (5n-2)(\sqrt{6}+\sqrt{8}) + (2n-1)(2\sqrt{8}) + n[7\sqrt{3} + 12 + 2\sqrt{3} + 9\sqrt{5} + 16\sqrt{6} + 17\sqrt{7} + 3\sqrt{8}] + (2+\sqrt{8})$.

Proof:

The ve-Sombor index for HAC is given by,

$$SO_{ve}(HAC) = \sum_{uw \in E} \sqrt{d_{ve}(u)^2 + d_{ve}(w)^2}$$

With the help of Table 1 we get,

$$\begin{aligned} SO_{ve}(HAC) = {} & (3n+1)\sqrt{2^2+4^2} + 2n\sqrt{3^2+4^2} + 2n\sqrt{3^2+5^2} + 3n\sqrt{3^2+7^2} \\ & + (6n+1)\sqrt{5^2+5^2} + \sqrt{8^2+4^2} + (9n-2)\sqrt{6^2+7^2} \\ & + (5n-2)\sqrt{6^2+8^2} + 3n\sqrt{7^2+4^2} + (n+2)\sqrt{5^2+7^2} + n\sqrt{6^2+4^2} \\ & + 3n\sqrt{6^2+6^2} + 7n\sqrt{5^2+6^2} + (2n-1)\sqrt{8^2+8^2} + 3n\sqrt{7^2+8^2} \\ & + 4n\sqrt{7^2+7^2} \end{aligned}$$

After simplifying we get the required result.

Similarly, one can easily prove the remaining results.

Theorem 3.1.2.Let HAP be the HA-paclitaxel conjugate. Then,

i. $SO_{ve}(HAP) = 2(n+1)\sqrt{5} + 6n[5 + 4\sqrt{2} + \sqrt{41}] + 4n[3\sqrt{5} + 6\sqrt{2} + \sqrt{113} + \sqrt{149}] + 5n[\sqrt{58} + 7\sqrt{2}] + n[\sqrt{73} + \sqrt{61} + \sqrt{89} + \sqrt{117} + \sqrt{136} + \sqrt{202}] + 2n[\sqrt{52} + \sqrt{65} + \sqrt{97} + \sqrt{116} + \sqrt{221}] + [\sqrt{80} + 5\sqrt{2}] + (6n+2)\sqrt{74} + (9n-2)\sqrt{85} + 10(10n-2) + 8(4n-1)\sqrt{2}$,

ii. $N_{ve}(HAP) = (n+1)\sqrt{6} + 6n[\sqrt{7} + \sqrt{8} + 3] + 4n[2\sqrt{3} + \sqrt{15} + \sqrt{17} + 3] + 5n[\sqrt{10} + \sqrt{14}] + n[2\sqrt{11} + \sqrt{13} + \sqrt{15} + \sqrt{20} + 4] + 2n[\sqrt{10} + \sqrt{11} + \sqrt{13} + \sqrt{14} + \sqrt{21}] + [\sqrt{12} + \sqrt{10}] + 2(6n+2)\sqrt{3} + (9n-2)\sqrt{15} + (10n-2)\sqrt{14} + 4(4n-1)$,

iii. $MPI_{ve}(HAP) = (n+1)[4] + 6n[8 + \sqrt{5} + \sqrt{3}] + 4n[\sqrt{3} + 3\sqrt{6} + 2\sqrt{7} + \sqrt{8} + \sqrt{10}] + 5n[\sqrt{3} + 3\sqrt{7}] + n[\sqrt{3} + 2\sqrt{8} + 2\sqrt{5} + 3\sqrt{6} + \sqrt{10} + \sqrt{11} + 6] + 2n[\sqrt{6} + \sqrt{7} + 2\sqrt{10} + \sqrt{11} + 11] + [2\sqrt{2} + 2\sqrt{5} + 2] + (6n+2)[\sqrt{5} + \sqrt{7}] + (9n-2)[\sqrt{6} + \sqrt{7}] + (10n-2)[\sqrt{6} + \sqrt{8}] + 2(4n-1)\sqrt{8}$.

Proof:The ve-Sombor index for HAC is given by,

$$SO_{ve}(HAC) = \sum_{uw \in E} \sqrt{d_{ve}(u)^2 + d_{ve}(w)^2}$$

With the help of Table 1 we get,

$$\begin{aligned} SO_{ve}(HAC) = {} & (n+1)\sqrt{2^2+4^2} + 6n\sqrt{3^2+4^2} + 4n\sqrt{3^2+6^2} + 5n\sqrt{3^2+7^2} \\ & + n\sqrt{3^2+8^2} + 6n\sqrt{4^2+4^2} + 6n\sqrt{4^2+5^2} + 2n\sqrt{4^2+6^2} + 2n\sqrt{4^2+7^2} \end{aligned}$$

$$+\sqrt{4^2+8^2}+2n\sqrt{4^2+9^2}+2n\sqrt{4^2+10^2}+\sqrt{5^2+5^2}+n\sqrt{5^2+6^2}$$
$$+(6n+2)\sqrt{5^2+7^2}+n\sqrt{5^2+8^2}+4n\sqrt{6^2+6^2}+\sqrt{5^2+5^2}+$$
$$(9n-2)\sqrt{7^2+6^2}+(10n-2)\sqrt{6^2+8^2}+n\sqrt{6^2+9^2}+n\sqrt{6^2+10^2}+$$
$$5n\sqrt{7^2+7^2}+4n\sqrt{7^2+8^2}+4n\sqrt{7^2+8^2}+4n\sqrt{7^2+10^2}+\ (4n-1)\sqrt{8^2+8^2}+$$
$$3n\sqrt{8^2+10^2}+3n\sqrt{9^2+10^2}+n\sqrt{9^2+11^2}+2n\sqrt{11^2+10^2}.$$

On simplifying the above equation, we get the required result. Through this, we can also get the remaining results.

4. Conclusions

In this study, we have computed SO_{ve}, N_{ve}, and MPI_{ve} of hyaluronic acid-curcumin/paclitaxel conjugate. The findings of the current studies will help the researchers better understand the physicochemical and pharmacological characteristics of hyaluronic acid-curcumin/paclitaxel conjugates. The result found are helpful in chemical and pharmaceutical science. The graphical comparison of SO_{ve}, N_{ve}, and MPI_{ve} for the hyaluronic acid-curcumin/paclitaxel conjugate are shown in Figure 3 and Figure 4. By that comparison, we can say the values of SO_{ve}, N_{ve}, and MPI_{ve} changes almost linearly with the iterations.

Funding

This research received no external funding.

Acknowledgments

The author would like to thank Dr. N.Narahari, Department of Mathematics, Tumkur university, for many useful suggestions.

Conflicts of Interest

The authors declare no conflict of interest.

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