



ARTICLE

## Some Topological Values of Supramolecular Chain of Different Complexes of N-Salicylidene-L-Valine

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### ABSTRACT

L-valine is a glycogen-type amino acid regarded among the necessary mammalian amino acids. This is an amino acid that is essential for protein synthesis. N-salicylidene-L-valine is gaining a lot of attention because of its unique structure and increased catalytic and cytotoxic activity. We explore the chain of supramolecular dialkyltin N-salicylidene-L-valine complexes 2, 3, and 4 to learn more about this structure and its features regarding topological indices. We computed the first and second Randić index, harmonic index, sum-connectivity index, atom-bond-connectivity index, geometric arithmetic index and reduced reciprocal Randić index of Supramolecular Chain of Different Complexes of N-Salicylidene-L-Valine. Furthermore, we present an analysis of such structures using specific examples, as well as a comparison of topological indices.

### KEYWORDS

Molecular compounds; supramolecular chains; topological indices

## 1 Introduction

Medicine manufacturing has grown rapidly in recent years and that has resulted in the production of an enormous number of novel drugs. Consequently, a considerable number of efforts is required to investigate the pharmacological, chemical, and biological properties of these recently synthesized drugs that makes this enormous workload much more clustered and fussier. Sufficient scientific assistance, equipment and reagents are necessary for the evaluation of their performance and shortcomings of the existing drugs. Furthermore, the lack of research funding in underdeveloped countries makes it further difficult to investigate the performance of these drugs. Literature suggests an inextricable relationship between the molecular structures of the drugs to their corresponding pharmacodynamic



and chemical properties. The identification of the topological indices by quantifying the measures of molecular structures of a drug, can help the pharmaceutical researchers to predict the therapeutic performance of that drug. Advantageously, this can reduce the efforts and time required to optimize the pharmacological, chemical, and biological performance of the drugs. Thus, the mathematical methods computing the topological indices are of great importance in predicting the pharmacological properties of drugs. For the computation studies regarding the evaluation of topological indices of a drug, the chemical structure of a medication is mathematically represented as a graph atom represented by vertex and bond between the atoms represented by an edge. Suppose a drug's structure represented by a graph  $G$ , with vertices (atoms) and edges (chemical bonds). Here, the topological index is a real-valued function used to transform the drug's molecular composition to specified numerical values that are unique to a particular molecular structure. Literature is enriched by many of the significant indices for assessment of the pharmacological and chemical properties of the molecules in the past 40 years. For example, the discovery of these topological indices has found their applications in molecular graphs, nano materials, pharmaceutical and engineering fields. In literature, the topological properties of the metal-organic compounds [1] engineered nanostructures [2,3], silicon carbide [4], titanium-based nanostructures [5], organic structures [6], nanotubes [7–9], etc., have been reported. The ABC indices [10,11] have employed for some chemical structures and predicting the performance of the dendrimers/honeycomb network in the terms of their topological indices [12].

Mammalian essential amino acid among the twenty-amino acids of the protein is Lv which is a glycogen. Several coordination modes towards metal ions and extraordinary coordination capacity has seen by a carboxylate ligand with a chiral Schiff base NsLv synthesize from salicylaldehyde and Lv. Such metal complexes bearing ligands have been extensively used for both laboratory scale research and industrial scale [13–17]. An effective reagent for DNA cleavage, enantio-selective reaction catalysts and chiral fluorescent molecular sensors are the potential applications of these chiral metal complexes. Organotin compounds have an extensive range of applications in medicines, Synthesis of chemical compounds, catalysis and material science [18]. Furthermore, carboxylate ligands in organotin complexes have attracted huge attention owing to their well diverse structures, high cytotoxic and catalytic activities [19–21]. Potential biological and optical properties have been reported for NsLv organotin complexes [16,22,23]. There are many chemical ways reported to synthesize them either with a potassium or oxide mixing a chlorine with sodium and potassium, or NsLv.

Let  $\vartheta$  be a simple, loopless, linked molecular graph with a set of vertex values  $V(\vartheta)$  and edge set  $E(\vartheta)$ . Order and size of molecular graph is shown by  $|V(\vartheta)| = r$  and  $|E(\vartheta)| = s$ . The degree  $d(v)$  of a vertex  $v$  is a total number of edges that are incident on it. A molecular descriptor, also referred as a topological structure index, is a mathematical formula that yields a numerical value associated with some molecular structure. The formulas for topological indices discussed in this article are listed below, along with their citations.

#### Definitions:

In 1975, the Chemist Milan Randić [24] proposed a topological index

$$R_1(\vartheta) = \sum_{rs \in E(\vartheta)} \frac{1}{d(r)d(s)} \quad (1)$$

$$R_2(\vartheta) = \sum_{rs \in E(\vartheta)} \frac{1}{\sqrt{d(r)d(s)}} \quad (2)$$

The expression of harmonic index [25] is,

$$H(\vartheta) = \sum_{rs \in E(\vartheta)} \frac{2}{d(r) + d(s)} \quad (3)$$

The expression of sum-connectivity index [26] is,

$$SCI(\vartheta) = \sum_{rs \in E(\vartheta)} \frac{1}{\sqrt{d(r) + d(s)}} \quad (4)$$

The expression of atom-bond-connectivity index [27] is,

$$ABC(\vartheta) = \sum_{rs \in E(\vartheta)} \sqrt{\frac{d(r) + d(s) - 2}{d(r)d(s)}} \quad (5)$$

The expression of geometric-arithmetic index [28] is,

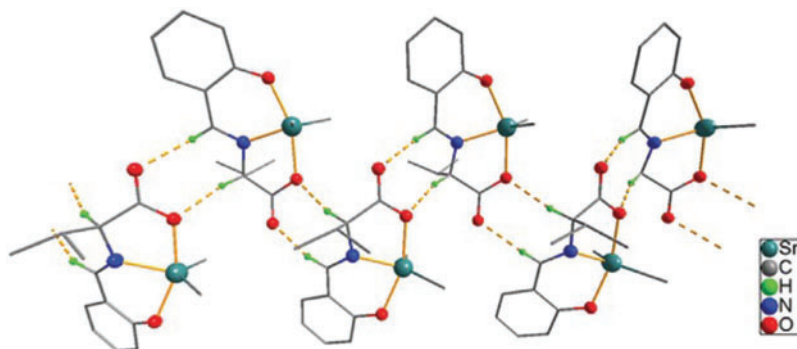
$$GA(\vartheta) = \sum_{rs \in E(\vartheta)} \frac{2\sqrt{d(r)d(s)}}{d(r) + d(s)} \quad (6)$$

The expression of reduced reciprocal Randić index [29] is,

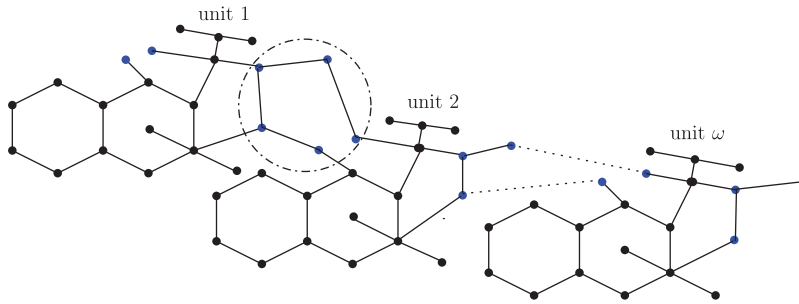
$$RRR(\vartheta) = \sum_{rs \in E(\vartheta)} \sqrt{(d(r) - 1)(d(s) - 1)} \quad (7)$$

## 2 Sc in Dialkyltin Complex-2 of NsLv ( $C_{2,\omega}$ )

The four forms of sc found in dialkyltin are complexes 2, 3, 4, and 5 of NsLv. This section will go over complex-2. Complex-2 of NsLv is one of the dialkyltin sc complexes  $\omega$  units that are identical, the second unit is blended with the aid of a vertex with the first unit, and its miles further producing a series of  $\omega$  units [30], Fig. 1 shows the molecular structure of this. Fig. 2 depicts the generalized  $\omega$  the unit graph of this molecular shape is derived from the chemical structure in discern 1 by [30]. This chain contains a variety of bonds, including single-degree, two-degree, three-degree, four-degree, and five-degree bonds (vertices). Additionally, Table 1 represents the edge type with their end vertices degree and also the number of repetitions (frequency) of that edge, which is very useful for our computations. The order and size of  $C_{2,\omega}$ , are  $|V(C_{2,\omega})| = 21\omega$ ,  $|E(C_{2,\omega})| = 25\omega - 2$ , respectively.



**Figure 1:** Chemical structure of the sc in NsLv dialkyltin complex-2



**Figure 2:** Sc in dialkyltin complex-2 of NsLv

**Table 1:** The edge type with there end vertex degree in  $(C_{2,\omega})$

$(d(u), d(v))$	Frequency	$(d(u), d(v))$	Frequency
(2, 2)	$4\omega - 1$	(3, 3)	$4\omega - 1$
(2, 3)	$6\omega - 2$	(1, 5)	$2\omega$
(1, 3)	$2\omega + 2$	(2, 5)	$\omega + 1$
(1, 4)	1	(3, 5)	$2\omega - 1$
(3, 4)	$3\omega$	(2, 4)	$\omega - 1$

**Theorem 2.1.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in NsLv dialkyltin complex-2 exists, then the first definition of the Randić index is,

$$R_1(C_{2,\omega}) = 4.112\omega + 0.125$$

**Proof.** By applying the first definition of the Randić index and [Table 1](#)

$$\begin{aligned}
 R_1(C_{2,\omega}) &= (4\omega - 1) \frac{1}{2 \times 2} + (6\omega - 2) \frac{1}{2 \times 3} + (2\omega + 2) \frac{1}{1 \times 3} + (1) \frac{1}{1 \times 4} \\
 &+ (3\omega) \frac{1}{3 \times 4} + (4\omega - 1) \frac{1}{3 \times 3} + (2\omega) \frac{1}{1 \times 5} + (\omega + 1) \frac{1}{2 \times 5} \\
 &+ (2\omega - 1) \frac{1}{3 \times 5} + (\omega - 1) \frac{1}{2 \times 4}.
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$R_1(C_{2,\omega}) = 4.112\omega + 0.125$$

**Theorem 2.2.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-2 exists, the harmonic index is,

$$H(C_{2,\omega}) = 9.375\omega - 0.53$$

**Proof.** By applying the expression of the harmonic index and [Table 1](#)

$$\begin{aligned}
 H(C_{2,\omega}) &= (4\omega - 1) \frac{2}{2+2} + (6\omega - 2) \frac{2}{2+3} + (2\omega + 2) \frac{2}{1+3} + (1) \frac{2}{1+4} \\
 &+ (3\omega) \frac{2}{3+4} + (4\omega - 1) \frac{2}{3+3} + (2\omega) \frac{2}{1+5} + (\omega + 1) \frac{2}{2+5} \\
 &+ (2\omega - 1) \frac{2}{3+5} + (\omega - 1) \frac{2}{2+4}.
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$H(C_{2,\omega}) = 9.375\omega - 0.53$$

**Theorem 2.3.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in NsLv dialkyltin complex-2 exists, then the second definition of the Randić index is,

$$R_2(C_{2,\omega}) = 9.877\omega - 0.29$$

**Proof.** By applying the second definition of the Randić index and [Table 1](#)

$$\begin{aligned}
 R_2(C_{2,\omega}) &= (4\omega - 1) \frac{1}{\sqrt{2 \times 2}} + (6\omega - 2) \frac{1}{\sqrt{2 \times 3}} + (2\omega + 2) \frac{1}{\sqrt{1 \times 3}} + (1) \frac{1}{\sqrt{1 \times 4}} \\
 &+ (3\omega) \frac{1}{\sqrt{3 \times 4}} + (4\omega - 1) \frac{1}{\sqrt{3 \times 3}} + (2\omega) \frac{1}{\sqrt{1 \times 5}} + (\omega + 1) \frac{1}{\sqrt{2 \times 5}} \\
 &+ (2\omega - 1) \frac{1}{\sqrt{3 \times 5}} + (\omega - 1) \frac{1}{\sqrt{2 \times 4}}.
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$R_2(C_{2,\omega}) = 9.877\omega - 0.29$$

**Theorem 2.4.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in NsLv dialkyltin complex-2 exists, then the sum-connectivity index is,

$$SCI(C_{2,\omega}) = 10.756\omega - 0.738$$

**Proof.** By applying the expression of the sum-connectivity index and [Table 1](#)

$$\begin{aligned}
 SCI(C_{2,\omega}) &= (4\omega - 1) \frac{1}{\sqrt{2+2}} + (6\omega - 2) \frac{1}{\sqrt{2+3}} + (2\omega + 2) \frac{1}{\sqrt{1+3}} + (1) \frac{1}{\sqrt{1+4}} \\
 &+ (3\omega) \frac{1}{\sqrt{3+4}} + (4\omega - 1) \frac{1}{\sqrt{3+3}} + (2\omega) \frac{1}{\sqrt{1+5}} + (\omega + 1) \frac{1}{\sqrt{2+5}} \\
 &+ (2\omega - 1) \frac{1}{\sqrt{3+5}} + (\omega - 1) \frac{1}{\sqrt{2+4}}.
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$SCI(C_{2,\omega}) = 10.756\omega - 0.738$$

**Theorem 2.5.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in NsLv dialkyltin complex-2 exists, then the Atom-Bond-Connectivity index is,

$$ABC(C_{2,\omega}) = 17.767\omega - 0.921$$

**Proof.** By applying the expression of the Atom-Bond-Connectivity index and [Table 1](#)

$$\begin{aligned} ABC(C_{2,\omega}) &= (4\omega - 1)\sqrt{\frac{2+2-2}{2 \times 2}} + (6\omega - 2)\sqrt{\frac{2+3-2}{2 \times 3}} + (2\omega + 2)\sqrt{\frac{1+3-2}{1 \times 3}} \\ &+ (1)\sqrt{\frac{1+4-2}{1 \times 4}} + (3\omega)\sqrt{\frac{3+4-2}{3 \times 4}} + (4\omega - 1)\sqrt{\frac{3+3-2}{3 \times 3}} + (2\omega)\sqrt{\frac{1+5-2}{1 \times 5}} \\ &+ (\omega + 1)\sqrt{\frac{2+5-2}{2 \times 5}} + (2\omega - 1)\sqrt{\frac{3+5-2}{3 \times 5}} + (\omega - 1)\sqrt{\frac{2+4-2}{2 \times 4}}. \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$ABC(C_{2,\omega}) = 17.767\omega - 0.921$$

**Theorem 2.6.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-2 exists, then the geometric-arithmetic index is,

$$GA(C_{2,\omega}) = 23.844\omega - 2.433$$

**Proof.** By applying the expression of the geometric-arithmetic index and [Table 1](#)

$$\begin{aligned} GA(C_{2,\omega}) &= (4\omega - 1)\frac{2\sqrt{2 \times 2}}{2+2} + (6\omega - 2)\frac{2\sqrt{2 \times 3}}{2+3} + (2\omega + 2)\frac{2\sqrt{1 \times 3}}{1+3} + (1)\frac{2\sqrt{1 \times 4}}{1+4} \\ &+ (3\omega)\frac{2\sqrt{3 \times 4}}{3+4} + (4\omega - 1)\frac{2\sqrt{3 \times 3}}{3+3} + (2\omega)\frac{2\sqrt{1 \times 5}}{1+5} + (\omega + 1)\frac{2\sqrt{2 \times 5}}{2+5} \\ &+ (2\omega - 1)\frac{2\sqrt{3 \times 5}}{3+5} + (\omega - 1)\frac{2\sqrt{2 \times 4}}{2+4}. \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$GA(C_{2,\omega}) = 23.844\omega - 2.433$$

**Theorem 2.7.** If  $C_{2,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-2 exists, then the reduced reciprocal Randić index is,

$$RRR(C_{2,\omega}) = 37.219\omega - 8.388$$

**Proof.** By applying the expression of the reduced reciprocal Randić index and [Table 1](#)

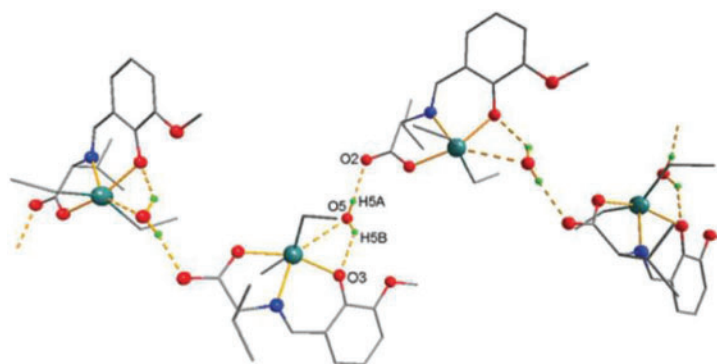
$$\begin{aligned} RRR(C_{2,\omega}) &= (4\omega - 1)\sqrt{(2-1)(2-1)} + (6\omega - 2)\sqrt{(2-1)(3-1)} + (2\omega + 2)\sqrt{(1-1)(3-1)} \\ &+ (1)\sqrt{(1-1)(4-1)} + (3\omega)\sqrt{(3-1)(4-1)} + (4\omega - 1)\sqrt{(3-1)(3-1)} \\ &+ (2\omega)\sqrt{(1-1)(5-1)} + (\omega + 1)\sqrt{(2-1)(5-1)} \\ &+ (2\omega - 1)\sqrt{(3-1)(5-1)} + (\omega - 1)\sqrt{(2-1)(4-1)}. \end{aligned}$$

After simplifying the previous equation, we get the following result:

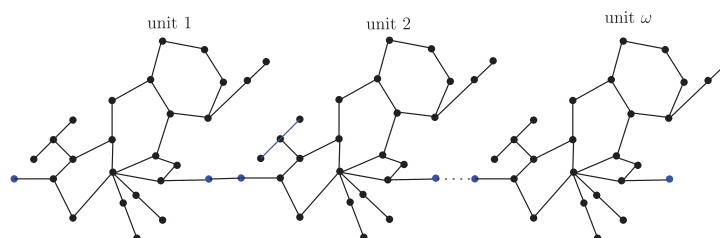
$$RRR(C_{2,\omega}) = 37.219\omega - 8.388$$

### 3 Sc in Dialkyltin Complex-3 of NsLv ( $C_{3,\omega}$ )

The sc in dialkyltin has four different forms of complexes, which are referred to as complexes 2, 3, 4, and 5 of NsLv. Complex-3 will be discussed in this section. Complex-3 of NsLv is one of the sc complexes in dialkyltin  $\omega$  same gadgets, where the second unit is joined via a vertex to the first unit, and it produces a sequence of  $\omega$  units, [Fig. 3](#) shows the molecular graph of this. [Fig. 4](#) displays the parameter  $\omega$  unit graph of this molecular structure generalised from the chemical structure [\[30\]](#). This chain comprises a variety of bonds, including single degree, 2, 3, and 6 degree bonds (vertices). Also, [Table 2](#) represents the sort of edge with their end vertices degree and also the number of repetition (frequency) of that edge which is very useful in support of our computational work. The order and size of  $C_{3,\omega}$ , are  $|V(C_{3,\omega})| = 26\omega$ ,  $|E(C_{3,\omega})| = 30\omega - 1$ , respectively.



**Figure 3:** Chemical structure of the sc in the NsLv dialkyltin complex-3



**Figure 4:** Sc in the dialkyltin complex-3 of NsLv

**Table 2:** The edge type with there end vertex degree in  $(C_{3,\omega})$ 

$(d(u), d(v))$	Frequency	$(d(u), d(v))$	Frequency
(1, 2)	$3\omega$	(1, 3)	$2\omega + 2$
(2, 3)	$10\omega - 2$	(2, 6)	$3\omega$
(2, 2)	$3\omega - 1$	(3, 6)	$3\omega$
(3, 3)	$6\omega$		

**Theorem 3.1.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the first definition of the Randić index is,

$$R_1(C_{3,\omega}) = 5.655\omega + 0.084$$

**Proof.** By applying the first definition of the Randić index and [Table 2](#)

$$R_1(C_{3,\omega}) = (3\omega) \frac{1}{1 \times 2} + (10\omega - 2) \frac{1}{2 \times 3} + (3\omega - 1) \frac{1}{2 \times 2} + (6\omega) \frac{1}{3 \times 3} \\ + (2\omega + 2) \frac{1}{1 \times 3} + (3\omega) \frac{1}{2 \times 6} + (3\omega) \frac{1}{3 \times 6}.$$

After simplifying the previous equation, we get the following result:

$$R_1(C_{3,\omega}) = 5.655\omega + 0.084$$

**Theorem 3.2.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the harmonic index is,

$$H(C_{3,\omega}) = 11.416\omega - 0.3$$

**Proof.** By applying the expression of the harmonic index and [Table 2](#)

$$H(C_{3,\omega}) = (3\omega) \frac{2}{1+2} + (10\omega - 2) \frac{2}{2+3} + (3\omega - 1) \frac{2}{2+2} + (6\omega) \frac{2}{3+3} \\ + (2\omega + 2) \frac{2}{1+3} + (3\omega) \frac{2}{2+6} + (3\omega) \frac{2}{3+6}.$$

After simplifying the previous equation, we get the following result:

$$H(C_{3,\omega}) = 11.416\omega - 0.3$$

**Theorem 3.3.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the second definition of the Randić index is,

$$R_2(C_{3,\omega}) = 12.422\omega - 0.162$$



**Proof.** By applying the second definition of the Randić index and [Table 2](#)

$$R_2(C_{3,\omega}) = (3\omega) \frac{1}{\sqrt{1 \times 2}} + (10\omega - 2) \frac{1}{\sqrt{2 \times 3}} + (3\omega - 1) \frac{1}{\sqrt{2 \times 2}} + (6\omega) \frac{1}{\sqrt{3 \times 3}} \\ + (2\omega + 2) \frac{1}{\sqrt{1 \times 3}} + (3\omega) \frac{1}{\sqrt{2 \times 6}} + (3\omega) \frac{1}{\sqrt{3 \times 6}}.$$

After simplifying the previous equation, we get the following result:

$$R_2(C_{3,\omega}) = 12.422\omega - 0.162$$

**Theorem 3.4.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the sum-connectivity index is,

$$SCI(C_{3,\omega}) = 13.207\omega - 0.394$$

**Proof.** By applying the expression of the sum-connectivity index and [Table 2](#)

$$SCI(C_{3,\omega}) = (3\omega) \frac{1}{\sqrt{1+2}} + (10\omega - 2) \frac{1}{\sqrt{2+3}} + (3\omega - 1) \frac{1}{\sqrt{2+2}} + (6\omega) \frac{1}{\sqrt{3+3}} \\ + (2\omega + 2) \frac{1}{\sqrt{1+3}} + (3\omega) \frac{1}{\sqrt{2+6}} + (3\omega) \frac{1}{\sqrt{3+6}}.$$

After simplifying the previous equation, we get the following result:

$$SCI(C_{3,\omega}) = 13.207\omega - 0.394$$

**Theorem 3.5.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the Atom-Bond-Connectivity index is,

$$ABC(C_{3,\omega}) = 20.927\omega - 0.489$$

**Proof.** By applying the expression of the Atom-Bond-Connectivity index and [Table 2](#)

$$ABC(C_{3,\omega}) = (3\omega) \sqrt{\frac{1+2-2}{1 \times 2}} + (10\omega - 2) \sqrt{\frac{2+3-2}{2 \times 3}} + (3\omega - 1) \sqrt{\frac{2+2-2}{2 \times 2}} \\ + (6\omega) \sqrt{\frac{3+3-2}{3 \times 3}} + (2\omega + 2) \sqrt{\frac{1+3-2}{1 \times 3}} + (3\omega) \sqrt{\frac{2+6-2}{2 \times 6}} + (3\omega) \sqrt{\frac{3+6-2}{3 \times 6}}.$$

After simplifying the previous equation, we get the following result:

$$ABC(C_{3,\omega}) = 20.927\omega - 0.489$$

**Theorem 3.6.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the geometric-arithmetic index is,

$$GA(C_{3,\omega}) = 28.77\omega - 1.226$$

**Proof.** By applying the expression of the geometric-arithmetic index and [Table 2](#)

$$GA(C_{3,\omega}) = (3\omega) \frac{2\sqrt{1 \times 2}}{1+2} + (10\omega - 2) \frac{2\sqrt{2 \times 3}}{2+3} + (3\omega - 1) \frac{2\sqrt{2 \times 2}}{2+2} + (6\omega) \frac{2\sqrt{3 \times 3}}{3 \times 3} \\ + (2\omega + 2) \frac{2\sqrt{1 \times 3}}{1+3} + (3\omega) \frac{2\sqrt{2 \times 6}}{2+6} + (3\omega) \frac{2\sqrt{3 \times 6}}{3+6}.$$

After simplifying the previous equation, we get the following result:

$$GA(C_{3,\omega}) = 28.77\omega - 1.226$$

**Theorem 3.7.** If  $C_{3,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-3 exist, then the reduced reciprocal Randić index is,

$$RRR(C_{3,\omega}) = 45.334\omega - 3.828$$

**Proof.** By applying the expression of the reduced reciprocal Randić index and [Table 2](#)

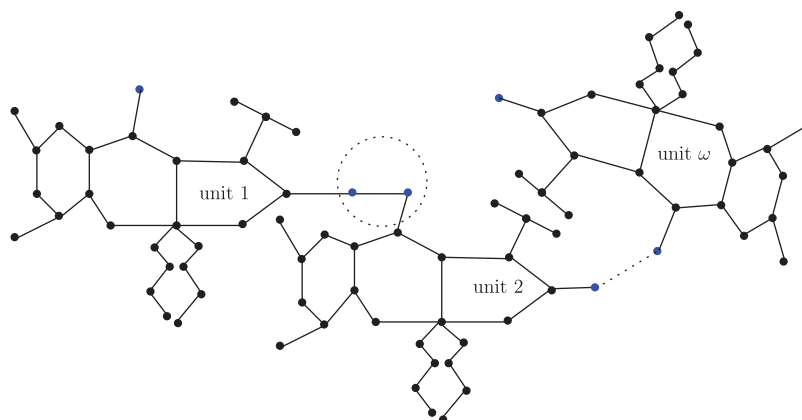
$$RRR(C_{3,\omega}) = (3\omega) \sqrt{(1-1)(2-1)} + (10\omega - 2) \sqrt{(2-1)(3-1)} + (3\omega - 1) \sqrt{(2-1)(2-1)} \\ + (6\omega) \sqrt{(3-1)(3-1)} + (2\omega + 2) \sqrt{(1-1)(3-1)} \\ + (3\omega) \sqrt{(2-1)(6-1)} + (3\omega) \sqrt{(3-1)(6-1)}.$$

After simplifying the previous equation, we get the following result:

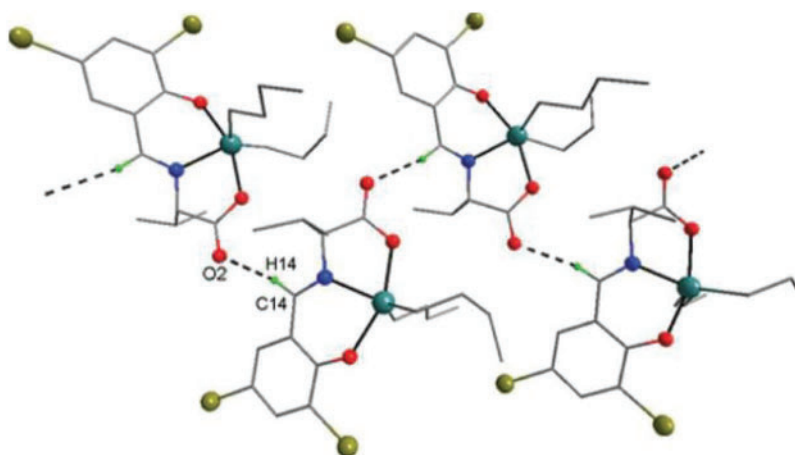
$$RRR(C_{3,\omega}) = 45.334\omega - 3.828$$

#### 4 Sc in Dialkyltin Complex-4 of NsLv ( $C_{4,\omega}$ )

The sc in dialkyltin has four different forms of complexes, which are referred as complexes 2, 3, 4, and 5 of NsLv. Complex-4 will be discussed in this section. Complex-4 of NsLv is one of the sc complexes in dialkyltin  $\omega$  equal devices, where the second one unit blended via a vertex with the first unit and its miles similarly developing with a sequence of parameter  $\omega$  units. [Fig. 5](#) suggests the generalized  $\omega$  unit graph of this molecular shape from the chemical structure given in [Fig. 6](#) by [30]. This chain comprises a variety of bonds, including single degree, 2, 3, and 5 degree bonds (vertices). Also, [Table 3](#) represents the edge type with their end vertices degree and also the number of repetition (frequency) of that edge which is very useful in support of our computation. The order and size of  $C_{4,\omega}$ , are  $|V(C_{4,\omega})| = 28\omega$ ,  $|E(C_{4,\omega})| = 31\omega - 1$ , respectively.



**Figure 5:** Sc in dialkyltin complex-4 of NsLv



**Figure 6:** Chemical structure of the sc in NsLv dialkyltin complex-4

**Table 3:** The edge type with there end vertex degree in  $(C_{4,\omega})$

$(d(u), d(v))$	Frequency	$(d(u), d(v))$	Frequency
(1, 3)	$4\omega + 2$	(2, 2)	$5\omega - 1$
(2, 3)	$8\omega - 2$	(2, 5)	$4\omega$
(3, 3)	$7\omega$	(3, 5)	$\omega$
(1, 2)	$2\omega$		

**Theorem 4.1.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the first definition of the Randić index is,

$$R_1(C_{4,\omega}) = 6.153\omega + 0.084$$

**Proof.** By applying the first definition of the Randić index and [Table 3](#)

$$R_1(C_{4,\omega}) = (4\omega + 2) \frac{1}{1 \times 3} + (8\omega - 2) \frac{1}{2 \times 3} + (7\omega) \frac{1}{3 \times 3} + (2\omega) \frac{1}{1 \times 2} \\ + (5\omega - 1) \frac{1}{2 \times 2} + (4\omega) \frac{1}{2 \times 5} + (\omega) \frac{1}{3 \times 5}.$$

After simplifying the previous equation, we get the following result:

$$R_1(C_{4,\omega}) = 6.153\omega + 0.084$$

**Theorem 4.2.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the harmonic index is,

$$H(C_{4,\omega}) = 12.759\omega - 0.3$$

**Proof.** By applying the expression of the harmonic index and [Table 3](#)

$$H(C_{4,\omega}) = (4\omega + 2) \frac{2}{1 + 3} + (8\omega - 2) \frac{2}{2 + 3} + (7\omega) \frac{2}{3 + 3} + (2\omega) \frac{2}{1 + 2} \\ + (5\omega - 1) \frac{2}{2 + 2} + (4\omega) \frac{2}{2 + 5} + (\omega) \frac{2}{3 + 5}.$$

After simplifying the previous equation, we get the following result:

$$H(C_{4,\omega}) = 12.759\omega - 0.3$$

**Theorem 4.3.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the second definition of the Randić index is,

$$R_2(C_{4,\omega}) = 13.339\omega - 0.162$$

**Proof.** By applying the second definition of the Randić index and [Table 3](#)

$$R_2(C_{4,\omega}) = (4\omega + 2) \frac{1}{\sqrt{1 \times 3}} + (8\omega - 2) \frac{1}{\sqrt{2 \times 3}} + (7\omega) \frac{1}{\sqrt{3 \times 3}} + (2\omega) \frac{1}{\sqrt{1 \times 2}} \\ + (5\omega - 1) \frac{1}{\sqrt{2 \times 2}} + (4\omega) \frac{1}{\sqrt{2 \times 5}} + (\omega) \frac{1}{\sqrt{3 \times 5}}.$$

After simplifying the previous equation, we get the following result:

$$R_2(C_{4,\omega}) = 13.339\omega - 0.162$$

**Theorem 4.4.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the sum-connectivity index is,

$$SCI(C_{4,\omega}) = 13.953\omega - 0.394$$

**Proof.** By applying the expression of the sum-connectivity index and [Table 3](#)

$$\begin{aligned}
 SCI(C_{4,\omega}) &= (4\omega + 2) \frac{1}{\sqrt{1+3}} + (8\omega - 2) \frac{1}{\sqrt{2+3}} + (7\omega) \frac{1}{\sqrt{3+3}} + (2\omega) \frac{1}{\sqrt{1+2}} \\
 &+ (5\omega - 1) \frac{1}{\sqrt{2+2}} + (4\omega) \frac{1}{\sqrt{2+5}} + (\omega) \frac{1}{\sqrt{3+5}}
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$SCI(C_{4,\omega}) = 13.953\omega - 0.394$$

**Theorem 4.5.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the Atom-Bond-Connectivity index is,

$$ABC(C_{4,\omega}) = 21.991\omega - 0.489$$

**Proof.** By applying the expression of the Atom-Bond-Connectivity index and [Table 3](#)

$$\begin{aligned}
 ABC(C_{4,\omega}) &= (4\omega + 2) \sqrt{\frac{1+3-2}{1 \times 3}} + (8\omega - 2) \sqrt{\frac{2+3-2}{2 \times 3}} + (7\omega) \sqrt{\frac{3+3-2}{3 \times 3}} \\
 &+ (2\omega) \sqrt{\frac{1+2-2}{1 \times 2}} + (5\omega - 1) \sqrt{\frac{2+2-2}{2 \times 2}} + (4\omega) \sqrt{\frac{2+5-2}{2 \times 5}} + (\omega) \sqrt{\frac{3+5-2}{3 \times 5}}.
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$ABC(C_{4,\omega}) = 21.991\omega - 0.489$$

**Theorem 4.6.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the geometric-arithmetic index is,

$$GA(C_{4,\omega}) = 29.761\omega - 1.226$$

**Proof.** By applying the expression of the geometric-arithmetic index and [Table 3](#)

$$\begin{aligned}
 GA(C_{4,\omega}) &= (4\omega + 2) \frac{2\sqrt{1 \times 3}}{1+3} + (8\omega - 2) \frac{2\sqrt{2 \times 3}}{2+3} + (7\omega) \frac{2\sqrt{3 \times 3}}{3+3} \\
 &+ (2\omega) \frac{2\sqrt{1 \times 2}}{1+2} + (5\omega - 1) \frac{2\sqrt{2 \times 2}}{2+2} + (4\omega) \frac{2\sqrt{2 \times 5}}{2+5} + (\omega) \frac{2\sqrt{3 \times 5}}{3+5}.
 \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$GA(C_{4,\omega}) = 29.761\omega - 1.226$$

**Theorem 4.7.** If  $C_{4,\omega}$ , with  $\omega \geq 1$  if a sc graph in the NsLv dialkyltin complex-4 exist, then the reduced reciprocal Randić index is,

$$RRR(C_{4,\omega}) = 41.14\omega - 3.828$$

**Proof.** By applying the expression of the reduced reciprocal Randić index and [Table 3](#)

$$\begin{aligned} RRR(C_{4,\omega}) &= (4\omega + 2) \sqrt{(1-1)(3-1)} + (8\omega - 2) \sqrt{(2-1)(3-1)} \\ &\quad + (7\omega) \sqrt{(3-1)(3-1)} + (2\omega) \sqrt{(1-1)(2-1)} + (5\omega - 1) \sqrt{(2-1)(2-1)} \\ &\quad + (4\omega) \sqrt{(2-1)(5-1)} + (\omega) \sqrt{(3-1)(5-1)}. \end{aligned}$$

After simplifying the previous equation, we get the following result:

$$RRR(C_{4,\omega}) = 41.14\omega - 3.828$$

## 5 Discussion

Topological indices are seen as a useful mechanism for investigating chemical characteristics and their own planned graphs through concepts of vertices and edges. The behaviour of a certain structure and graphs can be seen using topological indices, which provide numerical numbers. The current part compares seven degree based topological indices of our table-based structure, with matching graphs created by using a range of values 1 to 7 for the parameter  $\omega$  in the seventh topological indices. [Fig. 7](#) shows a plot of seven degree-based topological indices from the sc in dialkyltin complex-2 of NsLv ( $C_{2,\omega}$ ) made from the data in [Table 4](#). The plots grow in size in a linear pattern; the harmonic index, the second definition of the Randić index, and the sum-connectivity index are fairly close to each other, but the first definition of the Randić index moves extremely sharply among the others. [Fig. 8](#) shows a visualisation of seven degree-based topological indices for the structure of the sc in the NsLv dialkyltin complex-3 ( $C_{3,\omega}$ ) based on the values in [Table 5](#). The plots grow in size in a linear pattern; the harmonic index, the second definition of the Randić index, and the sum-connectivity index are fairly close to each other, but the first definition of the Randić index moves extremely sharply among the others. It is reasonable to believe that the first definition of the Randić index is more appropriate for studying our chosen structure than the others. [Fig. 9](#) shows a visualisation of seven degree-based topological indices for the structure of the sc in NsLv dialkyltin complex-4 ( $C_{4,\omega}$ ) based on the values in [Table 6](#). The plots grow in size in a linear pattern; the harmonic index, the second definition of the Randić index, and sum-connectivity index are fairly close to each other, but the first definition of the Randić index moves extremely sharply among the others. It is reasonable to believe that the first definition of Randić index is more appropriate for studying our chosen structure than the others.

Comparison of some indices for supramolecular chain in dialkyltin complex-2 of N-salicylidene-L-valine.

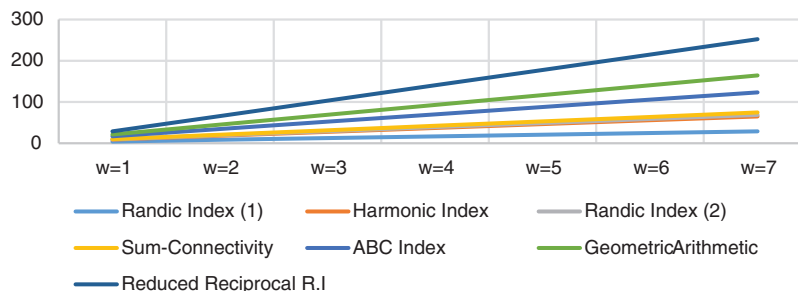


Figure 7: Correlation of some indices for sc in the dialkyltin complex-2 of NsLv

Table 4: Comparison of topological values in  $(C_{2,\omega})$

$\omega$	$R_1I$	$HI$	$R_2I$	$SCI$	$ABC$	$GA$	$RRR$
1	4.237	8.845	9.587	10.018	16.846	21.411	28.831
2	8.349	18.22	19.464	20.774	34.613	45.255	66.05
3	12.461	27.595	29.341	31.53	52.38	69.099	103.269
4	16.573	36.97	39.218	42.286	70.147	92.943	140.488
5	20.685	46.345	49.095	53.042	87.914	116.787	177.707
6	24.797	55.72	58.972	63.798	105.681	140.631	214.926
7	28.909	65.095	68.849	74.554	123.448	164.475	252.145

Comparison of some indices for supramolecular chain in dialkyltin complex-3 of N-salicylidene-L-valine.

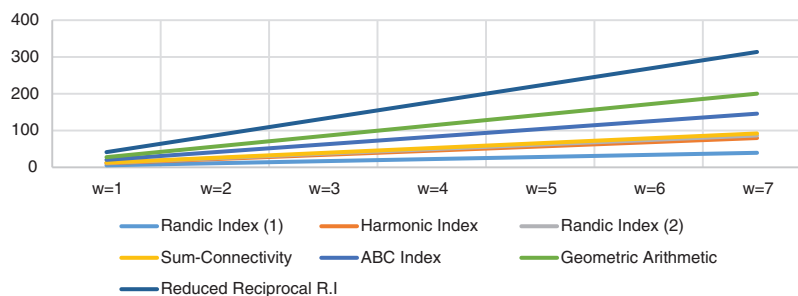
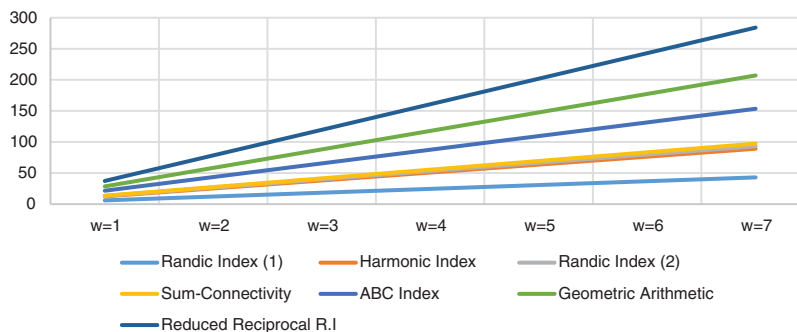


Figure 8: Correlation of some indices for sc in the dialkyltin complex-3 of NsLv

**Table 5:** Comparison of topological values in  $(C_{3,\omega})$ 

$\omega$	$R_1I$	$HI$	$R_2I$	$SCI$	$ABC$	$GA$	$RRR$
1	5.571	11.116	12.26	12.813	20.438	27.544	41.506
2	11.226	22.532	24.682	26.02	41.365	56.314	86.84
3	16.881	33.948	37.104	39.227	62.292	85.084	132.174
4	22.536	45.364	49.526	52.434	83.219	113.854	177.508
5	28.191	56.78	61.948	65.641	104.146	142.624	222.842
6	33.846	68.196	74.37	78.848	125.073	171.394	268.176
7	39.501	79.612	86.792	92.055	146	200.164	313.51

Comparison of some indices for supramolecular chain in dialkyltin complex-4 of N-salicylidene-L-valine.

**Figure 9:** Correlation of some indices for sc in the dialkyltin complex-4 of NsLv**Table 6:** Comparison of topological values in  $(C_{4,\omega})$ 

$\omega$	$R_1I$	$HI$	$R_2I$	$SCI$	$ABC$	$GA$	$RRR$
1	6.069	12.459	13.177	13.559	21.502	28.535	37.312
2	12.222	25.218	26.516	27.512	43.493	58.296	78.452
3	18.375	37.977	39.855	41.465	65.484	88.057	119.592
4	24.528	50.736	53.194	55.418	87.475	117.818	160.732
5	30.681	63.495	66.533	69.371	109.466	147.579	201.872
6	36.834	76.254	79.872	83.324	131.457	177.34	243.012
7	42.987	89.013	93.211	97.277	153.448	207.101	284.152

## 6 Conclusion

This study focused on chemical composition known as a sc in the dialkyltin complexes-2, 3, and 4 of NsLv using computational methods. To examine the behaviour of our chosen structures, we reviewed some relevant topological indices such as the first and second definitions of the Randić index,



the harmonic index, the sum-connectivity index, the abc index, the geometric-arithmetic index, and the reduced reciprocal Randić index. Furthermore, we conducted a comparative analysis by selecting specific values for an arbitrary parameter  $\omega$  associated to the structures and analysing them.

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