Bull. Chem. Soc. Ethiop. **2024**, 38(3), 647-655.
DOI: https://dx.doi.org/10.4314/bcse.v38i3.8

ISSN 1011-3924
Printed in Ethiopia
Online ISSN 1726-801X

BOOSTED ANTIBACTERIAL EFFICACY: DI AND TRIORGANOTIN COMPLEXES VIA 2-[(2,3-DIMETHYLPHENYL)AMINO]BENZOIC ACID

Rana S. Al-Shemary[1], Hadeer Jasem[2], Angham G. Hadi[3*] and Sadiq J. Baqir[4]

[1]Department of Pharmaceutical Chemistry, College of Pharmacy, University of Babylon, Babylon, Iraq
[2]Department of Physics, College of Education for Pure Sciences, University of Babylon, Iraq
[3]Department of Chemistry, College of Science, University of Babylon, Iraq
[4]Medical Laboratories Techniques Department, College of Health and Medical Techniques, Al-Mustaqbal University, 51001, Babylon Iraq

(Received December 4, 2023; Revised February 14, 2024; Accepted February 15, 2024)

ABSTRACT. Using appropriate organotin chloride salts and a ligand called 2-[(2,3-dimethylphenyl) amino] benzoic acid (DMPAB), a condensation procedure produced novel complexes such as triphenyltin, dimethyl, diphenyl, and dibutyl-tin. For difficult identification, a variety of analytical methods were used, including elemental analysis, carbon and proton magnetic resonance, and infrared spectra. The agar ditch method was used to assess the antibacterial effectiveness against *Staphylococcus aureus* and *Escherichia coli*. When compared to the molecule generated from the ligand, the complexes showed more inhibitory action. Among the complexes tested, the dimethyltin carboxylate complex showed the strongest antibacterial action against *Staphylococcus aureus* and *Escherichia coli.*

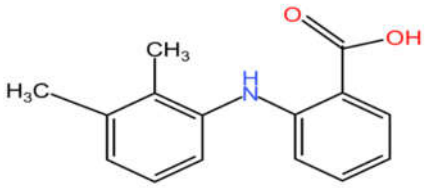
KEY WORDS: Complexes, Antibacterial properties, Condensation process, Agar Ditch, *Staphylococcus aureus* and *Escherichia coli*

INTRODUCTION

Organotin(IV) compounds are of great interest to the chemical and medicinal sectors. When producing pharmaceuticals that are biologically active molecules, tin(IV) produces stable complexes with unique structural, physical, and chemical features that are used as a catalyst and thermostat in organic synthesis. Organotin carboxylates are among the most significant categories of compounds [1]. Organotin carboxylates have theoretical and structural interests as well as practical applications in industry, the environment, and agriculture. [2-4]. In order to determine the optimal performance based on the ligand attached to the organometallic fragment and the origin, organotin(IV) compounds, in particular those derived from carboxylate ligands, have been thoroughly studied as bactericides [5-9], anti-cancer [10-12], antifungal and anti-inflammatory [13-15], catalysts, wood preservatives and pesticides [16]. The biological activities of organotin (IV) compounds are affected by both the length of the alkyl chain and the chemical structure of these compounds; the longer the alkyl chain, the less toxic the compound. [17-20], Aryl group-containing compounds are less poisonous than those without one, while triorganotin(IV) compounds—which have three Sn-C bonds—show the greatest cytotoxicity [21-25]. The synthesis of novel drugs using mineral complexes containing active pharmaceutical ingredients, such as ligands, is a rapidly developing field of study in inorganic and medicinal chemistry [26, 27]. In the last ten years, new drivers have been administered (NSAIDs) non-steroidal anti-inflammatory drugs and mineral compounds. Initially, due to their foundation in pure coordination chemistry. NSAIDs are a very adaptable coastline that, depending on the metal and surroundings, can offer a variety of bonding conditions. Certain complexes are interesting from a purely chemical perspective, or they exhibit greater biological activity or pharmacological than the

*Corresponding author. E-mail: sci.angam.ganem@uobabylon.edu.iq

medication [28-31]. The majority of NSAIDs, including aspirin, have a carboxyl group that can couple metal ions. The drugs of non-steroidal anti-inflammatory or NSAIDs, are frequently employed to deal with traumatic problems and inflammatory in together the rheumatic and non-rheumatic conditions. Examples of NSAIDs include 2-[(2,3-dimethylphenyl) amino] benzoic acid, tofenamic acid, and diclofenac sodium. 2-[(2,3-dimethylphenyl) amino] benzoic acid (DMPAB) is a commonly used analgesic medication in the market (Scheme 1).



Scheme 1. Chemical structure of 2-[(2,3-dimethylphenyl) amino] benzoic acid (DMPAB).

By using molecular techniques, we attempt to change the structure of (DMPAB) in order to get higher activity. In order to determine if there was an increase in antibacterial activity, the study focused on assessing the antibacterial properties of Sn(IV) compounds and comparing them with those of both (DMPAB) and the organic substituents derived from organotin(IV) compounds produced from (DMPAB).

EXPERIMENTAL

General

Chemicals were acquired from Merck (Schnelldorf, Germany). Melting points were determined with an MPD Mitamura Riken Kogyo apparatus (Tokushima, Japan). The elemental analyses were conducted with an EM-017mth instrument. Using KBr discs, FTIR spectra (400–4000 cm^{-1}) were recorded on an FTIR 8300 Shimadzu spectrophotometer (Tokyo, Japan). ^{1}H-(300 MHz), ^{13}C-(75 MHz), and ^{119}Sn-(107 MHz) NMR spectra were recorded on a Bruker DRX300 NMR spectrometer (Zurich, Switzerland).

*Di-organotin(IV) complexes **1–3** synthesis*

A methanol liquid (15 mL) containing 0.482 g (2 mmol) of DMPAB was continuously stirred for about 8 hours. Simultaneously, a hot solution of either di-butyltin, di-phenyltin, or di-methyltin salt (1 mmol) was slowly introduced into the reaction mixture. Diorganotin(IV) **1** , **2** or **3** was produced by recovering and recrystallizing the solid precipitate after it had cooled.

*Triorganotin(IV) complex **4** synthesis*

A quantity of 0.241 g, equivalent to one mmol of DMPAB, was slowly combined with a heated solution of triphenyltin chloride (10 mL) in methanol. The mixture refluxed for approximately eight hours. Triorganotin(IV) **4** was produced by recovering and recrystallizing the solid crystals after they had cooled.

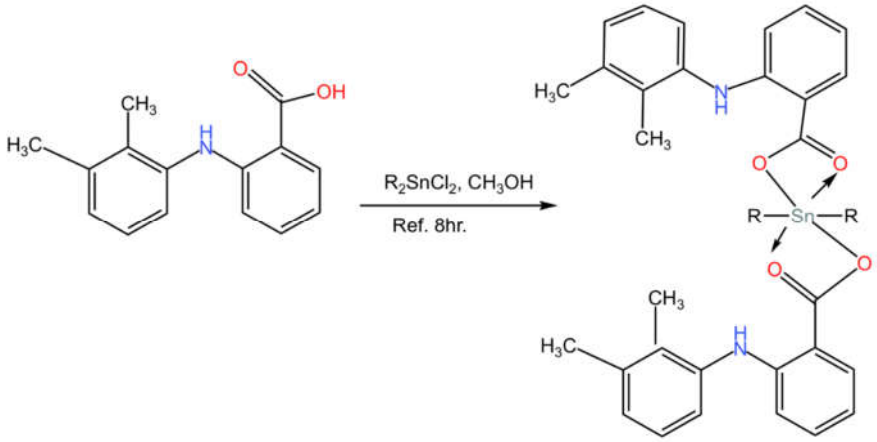
Biological activity

Applying the agar ditch method to *E. coli* and *S. aureus*, the antibacterial activity of several compounds was evaluated in vitro [32]. Each component was dissolved (40 mg) in 1 mL of ethanol to create the stock solutions, which were then used to create two-fold serial dilutions.

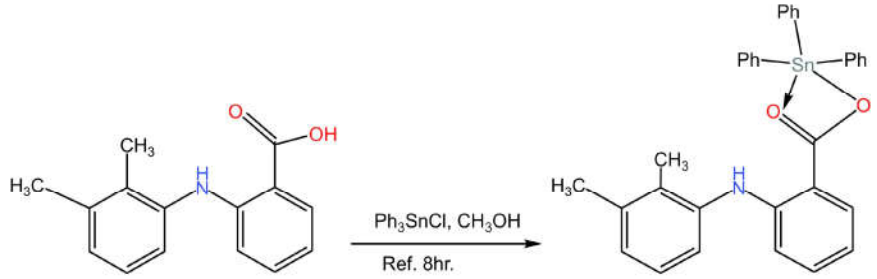
RESULTS AND DISCUSSION

*Di-organotin(IV) complexes **1–3** synthesis*

Conforming bis(DMPAB) Complexes involving di-organotin(IV) **1–3** were generated via a DMPAB reaction (2 mol equivalents) with Bu_2SnCl_2, Ph_2SnCl_2, or Me_2SnCl_2 undergo reflux in a methanol for a duration of around 8 hours. (Scheme 2). The yield percentages of these complexes were 17.5%, 27.08%, and 28.3%, respectively [2, 4].



Scheme 2. Diorganotin(IV) Complexes **1** , **2** and **3** Synthesis (R = Bu or Ph or Me).



Scheme 3. Triphenyltin(IV) complex **4**.

*Tri-organotin(IV) complexes **4** synthesis*

The matching (DMPAB) triorganotin(IV) complex **4** was produced with a 34.19% yield. A mixture containing equal molar amounts of DMPAB and triphenyl(IV) chloride was subjected to reflux in methanol for a duration of eight hours. (Scheme 3). Table 1 displays the physical parameters and elemental analysis of organotin(IV) complexes **1-4**.

Table 1. The CHN analysis and the physical properties of the synthesized complexes **1–4**.

Tin(IV) complex	R	Colour	% Yield	Melting point	Calcd. (Found); %		
					C	H	N
1	Bu_2	White	17.5	118-120	63.97 (62.88)	6.5 (6.23)	3.93 (3.57)
2	Ph_2	Light green	27.08	134-136	66.95 (65.69)	5.08 (6.15)	3.72 (3.1)
3	Me_2	White	28.30	213-215	61.07 (62.14)	5.45 (6.35)	4.45 (5.02)
4	Ph_3	White	34.19	123-125	67.14 (66.85)	4.95 (5.32)	2.37 (3.11)

*Infrared spectroscopy analysis of organotin(IV) complexes **1–4***

The FTIR spectra of Complexes **1–4** exhibit prominent peaks within the 521–525 cm^{-1} and 431–448 cm^{-1} ranges, respectively, corresponding to vibrations in the Sn–C and Sn–O groups [33]. Moreover, they exhibit strong absorption at 1653–1739 cm^{-1}, which is consistent with vibrations of the carbonyl group. Additional proof of the complexation is provided by the stretching vibration of the O-H group in the tin complexes disappearing, which first occurred at 3440 cm^{-1} for the ligand. Compounds **1-4**'s significant FTIR spectrum numbers are displayed in Table 2 and Figure 1.

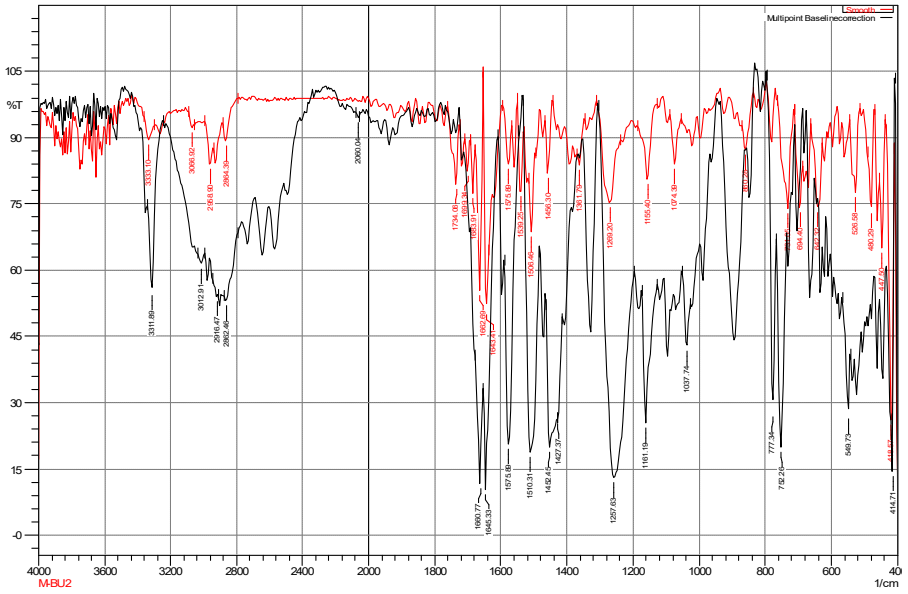


Figure 1. FTIR spectra of DMPAB and butyl complex.

Table 2. FTIR spectral data corresponding to complexes **1–4**.

Sn(IV) complex	FTIR (ν, cm^{-1})				
	N-H	C=O	C=C	Sn-C	Sn-O
1	3322	1652	1457	525	448
2	3312	1738	1457	521	431
3	3308	1661	1451	521	444
4	3312	1652	1453	523	447

*NMR spectroscopy of organotin(IV) complexes **1–4***

Organotin(IV) complexes **1-4** were confirmed to have their structures verified by NMR spectroscopy Figures 2 and 3. For every anticipated chemical shift, the NMR exhibits all expected signals (Table 3). Nevertheless, the ^{13}C-NMR spectra of **1-4** display several signals inside the aromatic region (Tables 3 and 4).

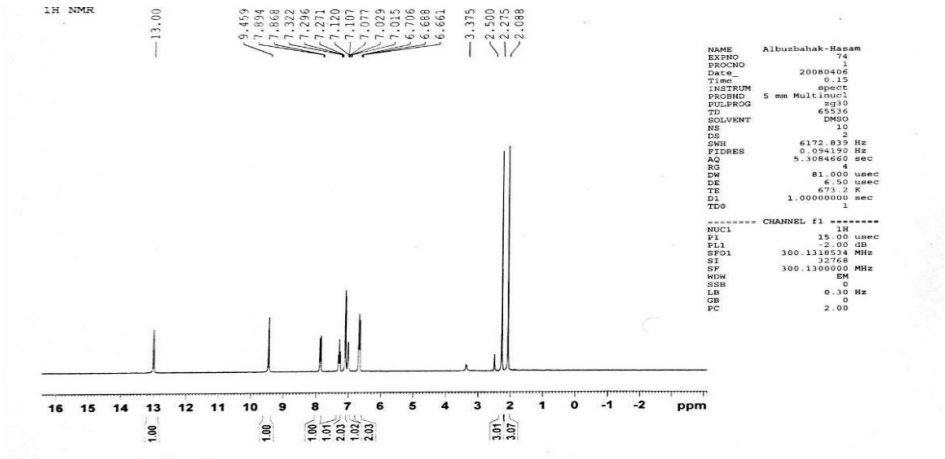


Figure 2. ^{1}H-NMR spectra of DMPAB.

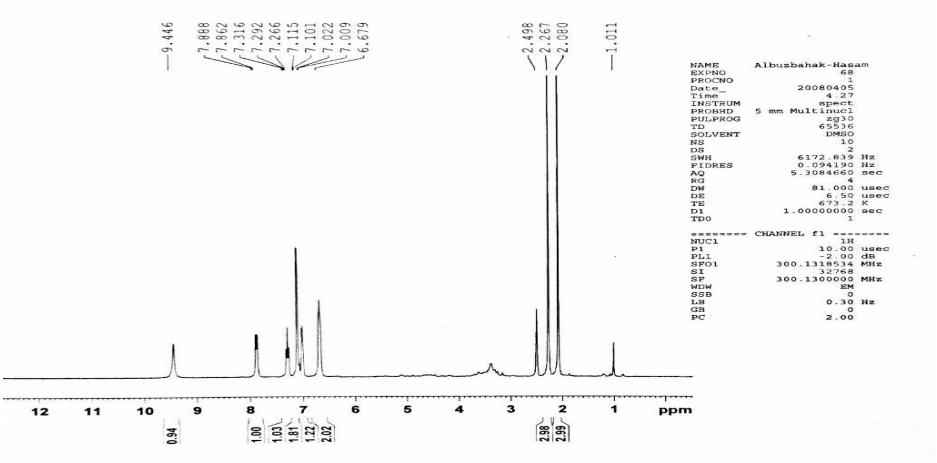


Figure 3. ^{1}H-NMR spectra of methyl complex.

Biological activity

The antibacterial activity was evaluated using the disc diffusion method. The microorganisms used were gram-positive (*Stuphylococcus aureus*) and gram-negative (*Escherichia coli*). Table 5 illustrates that the majority of the complexes that were evaluated had good antibacterial activity.

Table 3. ^{1}H-NMR spectral data for complexes **1–4**.

Sn(IV) complex	^{1}H-NMR
1	9.48 (s, H, NH), 6.68-7.98 (m, 6H, Aromatic), 2.51 (s, 3H, methyl), 2.05 (s, 3H, methyl), 1.87 (s, 2H, methylene), 1.45-1.71 (m, 5H, methylene) 0.81-0.88 (m, 2H, methyl).
2	9.55 (s, H, NH), 7.87-7.88 (m, 12H, Phenyl), 6.66-7.36 (m, 6H, Aromatic), 2.52 (s, 3H, methyl), 2.01 (s, 3H, methyl).
3	9.45 (s, H, NH), 6.68-7.89 (m, 6H, Ar), 2.48 (s, 3H, methyl), 2.18 (s, 3H, methyl), 1.02 (s, 3H, Me).
4	9.47 (s, H, NH), 7.84-7.87 (m, 18H, Phenyl), 6.67-7.49 (m, 6H, Aromatic), 2.51 (s, 3H, methyl), 2.08 (s, 3H, methyl).

Table 4. ^{13}C-NMR spectral information for complexes **1–4**.

Sn(IV) complex	^{13}C-NMR
1	171.71 (C=O), 149.22 (C-NH), 138.82 (C-NH), 138.32 (C-CH_3), 134.59, 132.18, 131.66, 126.83, 126.45, 122.6, 116.67, 113.52, 111.75, 34 (C-Sn), 28 (CH_2-Bu), 25 (CH_2-Bu), 14 (CH_3-Bu), 14.08 and 20.55 CH_3.
2	172.21 (carbonyl), 149.64 (C-N), 138.82 (C-N), 138.24 (C-methyl), 134.65, 132.20, 131.70, 126.88, 126.48, 122.66, 116.72, 113.55, 111.73, 14.11 and 20.67 CH_3.
3	172.24 (carbonyl), 149.65 (C-N), 138.34 (C-N), 138.45 (C-methyl), 134.64, 132.21, 131.70, 126.87, 126.48, 122.65, 116.72, 113.55, 111.73, 14.11 and 20.67 CH_3.
4	171.21 (carbonyl), 149.45 (C-N), 136.34 (C-N), 136.25 (C- methyl), 129.53, 129.48, 129.12, 128.90, 128.85, 128.80, 128.78, 128.57, 111.71, 14.14 and 20.54 CH_3.

Table 5. Antibacterial activity of compounds.

No.	Compound	G+ve *S. aureus*	G-ve *E. coli*
L	DMPAB	18	19
1	Bu_2	32	25
2	Ph_2	25	20
3	Me_2	35	30
4	Ph_3	30	26

Complex **3** (di methyltin–L) has the highest antibacterial property of all compounds when contrasted to the pure drug (DMPAB) [34]. This complex's stability, molecular configuration of the organotin(IV) compound , length of the alkyl chain, and the fact that complex **3** has more tin than the other complexes, which increases its antibacterial ability [35]. The synthesized complexes exhibit varying activity when compared to data in the literature because of variations in the cell wall structure. Gram negative cells have more intricate walls than gram positive cells [36]. In contrast to the *Stuphylococcus aureus,* which exhibit greater activities than *Escherichia coli* [37], For gram negative cells, the lipopolysaccharides create an outer lipid membrane and aid in complicated antigenic specificity [38]. This results in a decrease in the antibacterial activity of all complexes against *Escherichia coli.*

CONCLUSION

By using a condensation reaction between 2-[amino(2,3-dimethylphenyl)]benzoic acid (DMPAB) and tri- or di-tin salts, new organic tin complexes with a high yield ratio were created. Many techniques were used to identify these complexes, and after that, the possibility of employing

them as antibacterial agents was looked at. The synthesized complexes showed high biological activity in comparison to the ligands. Complex **3** (di methyltin–L) has the highest antibacterial property.

ACKNOWLEDGMENTS

The authors express their gratitude for the generous support provided by Babylon University and Al-Mustaqbal University College.

REFERENCES

1. Hadi, A.G.; Jawad, K.; Ahmed, D.S.; Yousif, E. Synthesis and biological activities of organotin (IV) carboxylates: A review. *Sys. Rev. Pharm.* **2018**, 1, 70-78.
2. Hadi, A.G.; Yousif, E.; El-Hiti, G.A.; Ahmed, D.S.; Jawad, K.; Alotaibi, M.H.; Hashim, H. Long-term effect of ultraviolet irradiation on poly (vinyl chloride) films containing naproxen diorganotin(IV) complexes. *Molecules* **2019**, 24, 2396.
3. Hadi, A.G.; Jawad, K.; El-Hiti, G.A.; Alotaibi, M.H.; Ahmed, A.A.; Ahmed, D.S.; Yousif, E. Photostabilization of poly (vinyl chloride) by organotin(IV) compounds against photodegradation. *Molecules* **2019**, 24, 3557.
4. Hadi, A.G.; Jawad, K.; Yousif, E.; El-Hiti, G.A.; Alotaibi, M.H.; Ahmed, D.S. Synthesis of telmisartan organotin(IV) complexes and their use as carbon dioxide capture media. *Molecules* **2019**, 24, 1631.
5. Adeyemi, J.O.; Onwudiwe, D.C.; Singh, M. Synthesis, characterization, and cytotoxicity study of organotin(IV) complexes involving different dithiocarbamate groups. *J. Mol. Struct.* **2019**, 1179, 366-375.
6. Syed Annuar, S.N.; Kamaludin, N.F.; Awang, N.; Chan, K.M. Cellular basis of organotin(IV) derivatives as anticancer metallodrugs: A review. *Front. Chem.* **2021**, 9, 657599.
7. Katsoulakou, E.; Tiliakos, M.; Papaefstathiou, G.; Terzis, A.; Raptopoulou, C.; Geromichalos, G.; Cordopatis, P. Diorganotin (IV) complexes of dipeptides containing the α-aminoisobutyryl residue (Aib): Preparation, structural characterization, antibacterial and antiproliferative activities of [(n-Bu)2Sn(H−1L)] (LH = H-Aib-L-Leu-OH, H-Aib-L-Ala-OH). *J. Inorg. Biochem.* **2008**, 102, 1397-1405.
8. Erfan, A.; Yousif, E.; Alshanon, A.N.; Ahmed, D.S.; Bufaroosha, M.; El-Hiti, G. Organotin(IV) complexes as promising potential drug candidates in the field of cancer chemotherapy: A narrative review. *Al-Rafidain J. Med. Sci.* **2023**, 5, 48-56.
9. Joshi, R.; Kumar, P.; Kumar, V.; Hashmi, A.A. Organotin(IV) oxo-homoscorpionate: preparation, spectroscopic characterization and antimicrobial properties. *J. Coord. Chem.* **2008**, 61, 1283-1293.
10. Debnath, P.; Debnath, P.; Roy, M.; Sieroń, L.; Maniukiewicz, W.; Misra, T.K. Novel organotin(IV) complexes of 2-[4-hydroxy-3-((2-hydroxyethylimino) methyl) phenylazo] benzoic acid: Synthesis, structure, noncovalent interactions and in vitro antibacterial activity. *Crystals* **2022**, 12, 1582.
11. Kovala-Demertzi, D.; Dokorou, V.; Primikiri, A.; Vargas, R., Silvestru; C., Russo, U.; Demertzis, M.A. Organotin meclofenamic complexes: Synthesis, crystal structures and antiproliferative activity of the first complexes of meclofenamic acid–novel anti-tuberculosis agents. *J. Inorg. Biochem.* **2009**, 103, 738-744.
12. Hadjikakou, S.K.; Hadjiliadis, N. Antiproliferative and anti-tumor activity of organotin compounds. *Coord. Chem. Rev.* **2009**, 253, 235-249.
13. Antonenko, T.A.; Gracheva, Y.A.; Shpakovsky, D.B.; Vorobyev, M.A.; Tafeenko, V.A.; Mazur, D.M.; Milaeva, E.R. Cytotoxic activity of organotin compounds containing non-steroidal anti-inflammatory drugs. *J. Organomet. Chem.* **2022**, 960, 122191.

14. Nath, M.; Pokharia, S.; Eng, G.; Song, X.; Kumar, A. New triorganotin(IV) derivatives of dipeptides as models for metal–protein interactions: Synthesis, structural characterization and biological studies. *Spectrochimica Acta Part A: Molecular Biomol. Spectrosc.* **2006**, 63, 66-75.
15. Rauf, M.K.; Saeed, M.A.; Bolte, M.; Badshah, A.; Mirza, B. Synthesis, characterization and biological activities of some new organotin(IV) derivatives: Crystal structure of [(Sn Ph_3)($OOCC_6H_4OH$)] and [($SnMe_3$)$_2$(OOC)$_2C_6Cl_4$($DMSO$)$_2$]. *J. Organomet. Chem.* **2008**, 693, 3043-3048.
16. Gonzalez, A.; Gomez, E.; Cortes-Lozada, A.; Hernández, S.; Ramírez-Apan, T.; Nieto-Camacho, A. Heptacoordinate tin(IV) compounds derived from pyridine Schiff bases: Synthesis, characterization, in vitro cytotoxicity, anti-inflammatory and antioxidant activity. *Chem. Pharm. Bull*. **2009**, 57, 5-15.
17. Carrera, N.; Gutiérrez, E.; Benavente, R.; Villavieja, M.M.; Albéniz, A.C.; Espinet, P. Stannylated polynorbornenes as new reagents for a clean Stille reaction. *Chem. Eur. J.* **2008**, 14, 10141-10148.
18. Dokorou, V.N.; Kovala-Demertzi, D.; Louloudi, M.; Silvestru, A.; Demertzis, M.A. Synthesis, characterization and catalytic properties of diorganotin derivatives. Crystal and molecular structure of the first complex of 2-(2-methyl-3-nitroanilino) benzoic acid of 1, 2: 3, 4-di-μ2-2-(2-methyl-3-nitroanilino) benzoato-O,o-1, 3-bis-2-(2-methyl-3-nitroanilino) benzoato-O-1, 2, 4: 2, 3, 4-di-μ3-oxo-tetrakis [di-methyltin(IV)]. *J. Organomet. Chem.* **2008**, 693, 3587-3592.
19. Van Kerk, G.D.; Luijten, J.G.A. Investigations on organo-tin compounds. III. The biocidal properties of organo-tin compounds. *J. Appl. Chem.* **1954**, 4, 314-319.
20. van der Kerk, G.J.M.; Luijten, J.G.A. Investigations on organo-tin compounds. V The preparation and antifungal properties of unsymmetrical tri-n-alkyltin acetates. *J. Appl. Chem.* **1956**, 6, 56-60.
21. Song, X.; Zapata, A.; Eng, G. Organotins and quantitative-structure activity/property relationships. *J. Organomet. Chem.* **2006**, 691, 1756-1760.
22. Blunden, S.J. Organotin compounds in the environment. *Organometllic Compound in the Environment*, John Wiley & Sons, Ltd: Online publication; **1986**; pp. 111-159.
23. Nguyen, V.V.; Posey, I.J.; Eng, G. Speciation of antifoulant organotin compounds in water. *Water Air Soil Pollut.* **1984**, 23, 417-422.
24. Doctor, S.V.; Fox, D.A. Effects of organotin compounds on maximal electroshock seizure (MES) responsiveness in mice. I. Tri (n-ALKYL) tin compounds. *J. Toxicol. Environ. Healt.* **1982**, 10, 43-52.
25. Mushak, P.; Krigman, M.R.; Mailman, R.B. Comparative organotin toxicity in the developing rat: somatic and morphological changes and relationship to accumulation of total tin. *Neurobehav. Toxicol. Teratol.* **1982**, 4, 209-215.
26. Cini, R. Anti-inflammatory compounds as ligands in metal complexes as revealed in X-ray structural studies. *Comments Inorg. Chem.* **2000**, 22, 151-186.
27. Kovala-Demertzi, D. Transition metal complexes of diclofenac with potentially interesting anti-inflammatory activity. *J. Inorg. Biochem.* **2000**, 79, 153-157.
28. Ramadan, S.; Hambley, T.W.; Kennedy, B.J.; Lay, P.A. NMR spectroscopic characterization of copper(II) and zinc(II) complexes of indomethacin. *Inorg. Chem.* **2004**, 43, 2943-2946.
29. Theodorou, A.; Demertzis, M.A.; Kovala-Demertzi, D.; Lioliou, E.E.; Pantazaki, A.A.; Kyriakidis, D.A. Copper(II) complexes of diclofenac: Spectroscopic studies and DNA strand breakage. *BioMetals*. **1999**, 12, 167-172.
30. Abuhijleh, A.L.; Woods, C. Mononuclear copper(II) salicylate imidazole complexes derived from copper(II) aspirinate. Crystallographic determination of three copper geometries in a unit cell. *Inorg. Chem. Commun.* **2001**, 4, 119-123.

31. Kovala-Demertzi, D. Recent advances on non-steroidal anti-inflammatory drugs, NSAIDs: organotin complexes of NSAIDs. *J. Organomet. Chem.* **2006**, 691, 1767-1774.
32. Rehder, D. Biological and medicinal aspects of vanadium. *Inorg. Chem. Commun*. **2003**, 6, 604-617.
33. Akram, M.A.; Nazir, T.; Taha, N.; Adil, A.; Sarfraz, M.; Nazir, S.R. Designing, development and formulation of mouth disintegrating telmisartan tablet with extended release profile using response surface methodology. *J. Bioequivalence Bioavailab.* **2015**, 7, 262.
34. Hashim, D.J.; Waheed, E.J.; Hadi, A.G.; Baqir, S.J. Exploring the biological activity of organotin carboxylate complexes with 4-sulfosalicylic acid. *Bull. Chem. Soc. Ethiop.* **2023**, 37, 1435-1442.
35. Hashim, D.J.; Al-Rikabi, E.H.; Hadi, A.G.; Baqir, S.J. 4-Aminoantipyrine-new organotin complexes, synthesis, structure and antioxidant activity. *Bull. Chem. Soc. Ethiop.* **2023**, 37, 1163-1170.
36. Singh, R.V.; Chaudhary, P.; Chauhan, S.; Swami, M. Microwave-assisted synthesis, characterization and biological activities of organotin(IV) complexes with some thio Schiff bases. *Spectrochim. Acta A Mol. Biomol.* **2009**, 72, 260-268.
37. Sharma, A.K.; Chandra, S. Complexation of nitrogen and sulphur donor Schiff's base ligand to Cr(III) and Ni(II) metal ions: Synthesis, spectroscopic and antipathogenic studies. *Spectrochim. Acta A Mol. Biomol.* **2011**, 78, 337-342.
38. Shahzadi, S.; Shahid, K.; Ali, S.; Mazhar, M.; Khan, K.M. Organotin(IV) derivatives as biocides: An investigation of structure by IR, solution NMR, electron impact MS and assessment of structure correlation with biocidal activity. *J. Iran. Chem. Soc.* **2005**, 2, 277-288.