# SYNTHESIS, CHARACTERIZATION, THEORETICAL MODELLING, AND BIOLOGICAL ASSESSMENT OF DIORGANOTIN(IV) COMPLEXES WITH THIAZOLE INCORPORATING AZO-SCHIFF BASE LIGANDS

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## Introduction

Organotin(IV) compounds ($R_nSnX_{n-1}$, where n = 1, 2, or 3) are well known for their diverse biological activities;

- Antimicrobial
- Anti-inflammatory
- Antioxidant
- Anticancer
- Cytotoxic
- Antimalarial
- Antituberculosis
- Antiviral

The incorporation of azo-Schiff base ligands can enhance the stability, reactivity, and bioavailability of organotin complexes, making them attractive candidates for medicinal applications.

While thiazole-containing derivatives are especially notable for their broad pharmacological potential.

Therefore, novel thiazole-based azo-Schiff base ligands ($ASbL_{1-4}$) were synthesized and successfully coordinated with dimethyltin(IV) and dibutyltin(IV) centers to afford eight new organotin(IV) complexes.

## Objective Alignment with SDG 3

This research supports the United Nations Sustainable Development Goal 3 (Good Health and Well-Being) by developing noveltherapeutic agents that may help combat infectious diseases and inflammation-related disorders, ultimately promoting improved health outcomes.

## Synthetic Route

**Step 1**

Schiff base formation from 3,5-dichlorosalicylaldehyde and 2-aminophenol

**Step 2**


Azo formation from Schiff base via coupling reaction with respective thiazole derivatives

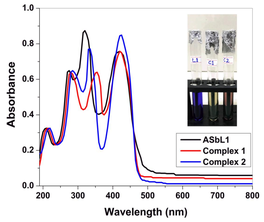
**Step 3**

Complex formation by mixing Azo-Schiff base ligand and respective tin(IV) salts

ASbL1 → 2-aminothiazole
ASbL2 → 2-amino-5-nitrothiazole
ASbL3 → 2-aminobenzothiazole
ASbL4 → 2-amino-6-nitrobenzothiazole

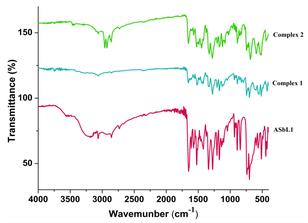
## Structural Characterizations of tin(IV) complexes

### UV-Visible



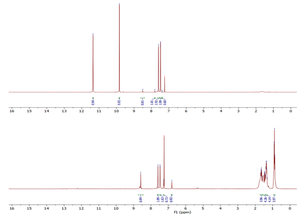

- π→π*, n→π*
- LMCT band observed
- Bathochromic shift after complexation

### FT-IR



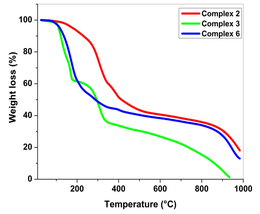

- Disappearance of phenolic –OH bands after coordination
- New Sn-O and Sn-N bands confirmed coordination

### $^1$H NMR



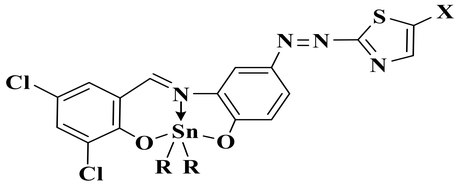
- Loss of phenolic –OH signals after Sn-O bonding
- Upfield shift of (HC=N) group
- Signals of $CH_3$/*n*-Bu in tin-spectra

### TGA




- Multi-step decomposition
- Final residue $SnO_2$
- No coordinated water molecule

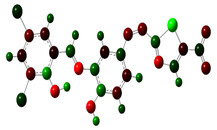
## Proposed Coordination Mode



X= H, $NO_2$
R= Me, *n*-Bu

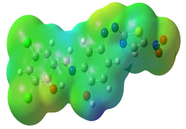
## Density Functional Theory

### Mulliken charges



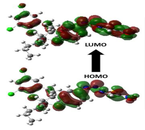
High negative charge density on phenolic –OH and imine N atoms

### MEP



Red = electron-rich region (N &O atoms)
Blue = electron-poor region (H atom)

### FMOs



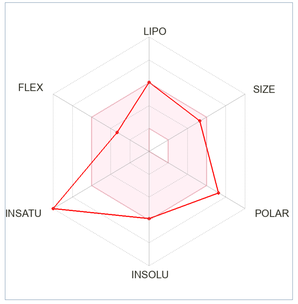

ΔE Ligands (2.48-2.88 eV)
ΔE Complexes (2.76-3.20)

Complexes have lower ΔE → Higher reactivity and better biological interaction

## SWISS ADME

Drug-Likeness (Lipinski's Rule)

- Molecular Weight < 500
- H-bond acceptors ≤ 10
- H-bond donors ≤ 5
- Log p < 5




Poorly soluble in water (mostly)
Good bioavailability score
NO CYP2D6 inhibition predicted
Acceptable TPSA, molar refractivity, GI absorption, BBB permeability

## Conclusion

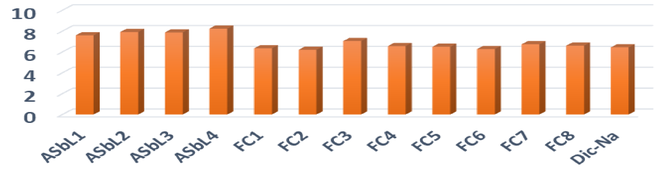
Novel thiazole-based azo ligands and their organotin(IV) complexes were successfully synthesized and characterized by various physicochemical techniques. The organotin(IV) complexes exhibited enhanced biological activities and favorable drug-like properties, highlighting their potential for future therapeutic applications.

## References


- P. Barwa, et al., Integrated experimental and theoretical studies of organotin (IV)-Hydrazone complexes: synthesis, structural elucidation, computational insights, and antimicrobial activity, Chem. Biodivers. 22 (9) (2025) e202500544.
- [104] M. Saeed, et al., Synthesis, characterization, in vitro and in silico biological studies of 3d transition metal (II) chelates of a schiff base derived from sulfamethazine and 3, 5-diiodosalicylaldehyde, J. Coord. Chem. 77 (15–16) (2024) 1860–1886.


## Biological Activities (Summary)

### Anti-Inflammatory Activity (Egg Albumin Method)

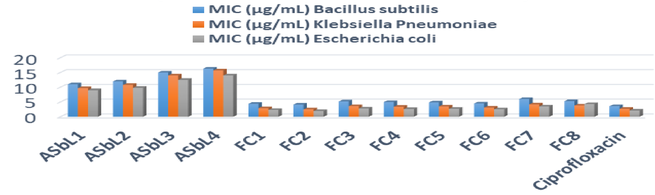



Organotin(IV) Complexes 1, 2, and 4 showed activity better than Sodium Diclofenac (IC50 = 6.44 µM)

### Antioxidant Activity (DPPH assay)


Organotin(IV) Complexes exhibited stronger radical scavenging activity (best Complex 4, IC50 = 3.01 µM)

### Antibacterial Activity (Disc Diffusion Method)




Diorganotin(IV) Complexes > azo Schiff-base ligands
Dibutyltin(IV) complexes > dimethyltin(IV) complexes
More susceptible to Gram-negative bacteria