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FULL PAPER

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Synthesis, characterization, biological screening and molecular docking of Zn(II) and Cu(II) complexes of 3,5-dichlorosalicylaldehyde-N^4-cyclohexylthiosemicarbazone

Nimya Ann Mathews[1] | **P.M. Sabura Begum**[1] | **M.R. Prathapachandra Kurup**[1,2]

[1]Department of Applied Chemistry, Cochin University of Science and Technology, Kochi 682 022Kerala, India

[2]Department of Chemistry, School of Physical Sciences, Central University of Kerala, Tejaswini Hills, Periye, Kasaragod 671 320, India

Correspondence
M. R. Prathapachandra Kurup, Department of Chemistry, School of Physical Sciences, Central University of Kerala, Tejaswini Hills, Periye. Kasaragod, 671 320, India.
Email: mrpcusat@gmail.com

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A 3,5-dichlorosalicylaldehyde-N^4-cyclohexylthiosemicarbazone ($C_{14}H_{16}Cl_2N_3OS$) and its complexes [Zn(dsct)(phen)]·DMF (**1**), [Zn(dsct)(bipy)]·DMF (**2**), [Cu(dsct)(bipy)]·DMF (**3**) (phen = 1,10-phenathroline, bipy = 2,2'bipyridine) were synthesized and characterized by CHN analysis, FT-IR, UV–vis and NMR spectra. The molecular structure of the thiosemicarbazone (H_2dsct) and its complexes have been resolved using single crystal XRD studies. In the complexes, thiosemicarbazone exist in the thioiminolate form and acts as dideprotonated tridentate ligand coordinating through phenolic oxygen, thioiminolate sulfur and azomethine nitrogen. The antibacterial activity of the prepared compounds were screened against *Escherichia coli*, *Salmonella typhi, Enterobacter aerogenes, Shigella dysentriae, Bacillus cereus, Staphylococcus aureus*. All the complexes showed activity against bacterial strains *E.coli* and *Salmonella typhi*. The thiosemicarbazone showed activity against three bacterial strains such as *E. coli, Enterobacter aerogenes* and *Shigella dysentriae*. Complex **2** showed very good antibacterial activity as compared to standard drug (Ampicillin) against the bacterial strain, *Salmonella typhi*. Finally, the thiosemicarbazone and its complexes have been used to accomplish molecular docking studies against an Epidermal Growth Factor Receptor (EGFR) and breast cancer mutant 3hb5-oxidoreductase to determine the most preferred mode of interaction. The results confirm that the complex [Cu (dsct)(bipy)]·DMF(**3**) showed the highest docking score as compared to other complexes under study. The [Cu(dsct)(bipy)]·DMF(**3**) complex was evaluated for their anticancer activities against breast cancer cell line (MCF-7) and normal L929 (Mouse Fibroblast) cell line. It was found that the compound showed an LC_{50} of 6.25 μg/mL against breast cancer cell line (MCF-7).

KEYWORDS
antibacterial activity, crystal structures, molecular docking, MTT, Thiosemicarbazones

1 | INTRODUCTION

Thiosemicarbazones are a class of Schiff base compound of chelating bio ligands that contain a thiourea moiety and they attract considerable attention due to their ease of preparation, excellent complexation, variety of coordination modes and useful pharmacological properties and pharmacological applications.[1,2] They are versatile ligands and efficient metal chelators. A number of reasons have been responsible for the versatility in their

