

**Frontiers in Pharmaceutical, Material, and
Environmental Sciences: Innovative Approaches
and Applications**

Editors

Tahmeena Khan

Qazi Inamur Rahman

Nafees Ahmad

Shahla Tanveer

*Department of Chemistry,
Integral University, Lucknow*



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PREFACE

This book brings together a collection of research studies that delve into the fields of pharmaceutical science, materials science, and environmental science. The chapters within this volume highlight innovative methods and significant discoveries in these areas. The research presented here explores the development of advanced drug delivery systems, the therapeutic potential of natural products, the removal of environmental pollutants, and the optimization of material properties. By combining experimental techniques with computational modeling, the authors have gained deeper insights into the underlying mechanisms of these processes. We hope this book will serve as a valuable resource for researchers, academics, and industry professionals in these fields. The knowledge and insights provided here will contribute to the advancement of scientific research and the development of sustainable solutions for global challenges.

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Chapter – 10

Synthesis and Characterization of some Thiosemicarbazones and their Complexes

Atiya Khan¹, Tahmeena Khan^{1*}

Department of Chemistry, Integral University, Lucknow, U.P., India

Corresponding email: tahminakhan30@yahoo.com

Abstract

This chapter reports the synthesis and characterization of complexes of copper (II) and iron (II) with thiosemicarbazones of 2,4-dichlorothiosemicarbazone $[\text{Cu}(\text{C}_8\text{H}_7\text{Cl}_2\text{N}_3\text{S})_2]\text{SO}_4$, $[\text{Fe}(\text{C}_8\text{H}_7\text{Cl}_2\text{N}_3\text{S})_2]\text{SO}_4$ and salicylaldehyde thiosemicarbazone $[\text{Cu}(\text{C}_8\text{H}_9\text{N}_3\text{OS})_2]\text{SO}_4$, $[\text{Fe}(\text{C}_8\text{H}_9\text{N}_3\text{OS})_2]\text{SO}_4$ have been described. The ligands and complexes were prepared through refluxing. The characterization was done by FT-IR, UV, and NMR spectroscopic techniques. The physicochemical parameters of the synthesized ligand and complexes were calculated using Molinspiration and SwissADME, Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) properties were assessed using admetSAR. Physicochemical characteristics of synthesized ligands and their metal complexes were determined using Mol inspiration and SwissADME softwares. Properties like molecular weight topological polar surface area (TPSA), number of hydrogen bond donors and acceptors etc. were calculated to know the probable potential of molecules as lead candidates. TPSA was within the range i.e. below 102.73 Å and the number of hydrogen bond donors and acceptors were also within the suggested range.

Keywords: Thiosemicarbazones, virtual screening, SWissADME, Molinspiration