Dedicated
to
My Beloved Parents

MOSARRAF HOSSAIN

SIULI BIBI

DECLARATION

I, **Sahin Reja**, hereby declare that the work presented in this thesis entitled "Polydentate ligand based metal complexes for oxidase activity" is an authentic record of research work done by me under the supervision of Dr. Rajesh Kumar Das, Assistant Professor, Department of Chemistry, University of North Bengal, Darjeeling, West Bengal, India

The research work in this thesis (in full) has not been submitted elsewhere earlier, for the award of any other degree, diploma and fellowship to this or any other University/Institute.

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CERTIFICATE

This is to certify that the thesis entitled **"Polydentate ligand based metal complexes for oxidase activity"** is an authentic record of research work carried out by **Mr. Sahin Reja** for fulfilment of the requirements for the degree of "DOCTOR OF PHILOSOPHY IN CHEMISTRY" under my supervision at University of North Bengal, Darjeeling, West Bengal, India. I further certify that this research work is original, and no part of this thesis has been submitted for the award of any degree or diploma to this or any other University/Institute.

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PREFACE

I started the research work presented in this thesis entitled "Polydentate ligand based metal complex for oxidase activity" in the year 2019 under the supervision of Dr. Rajesh Kumar Das in the Department of Chemistry, University of North Bengal, India. In recent years, the study of metal complexes with polydentate ligands has gained significant attention due to their potential applications in various fields, such as catalysis, biological activity, and materials science. Among them, metal complexes with polydentate ligands have been found to exhibit remarkable oxidase activity, making them a promising candidate for developing efficient and selective oxidase mimics.

The thesis starts with ***Chapter I*** *where a detailed study of different types of ligands, metal complexes, oxidase activity and biological activity are described.* ***Chapter II*** *discusses all the methodologies associated with synthesis of ligand and metal complexes techniques in detail. A novel compound, 3-(1,3-dioxoisoindolin-2-yl)-N,N-dimethyl propan-1-aminium perchlorate (DIDAP), was successfully synthesized and characterized through various spectroscopic techniques, including single crystal X-ray diffraction, as discussed in* ***Chapter III****. DIDAP was found to self-assemble into a helical structure with strong intermolecular interactions in its solid state and exhibited promising anticancer activity against the Hep G2 cell line, supported by docking studies and computational analysis of its chemical reactivity.* ***Chapter IV*** *encompasses a novel compound, 3,3'-[succinylbis(diazaneyl)]bis(N,N,N-trimethylpropan-1-ammonium) perchlorate (SAPAP), synthesized from N1, N4- Bis(3-(dimethylamino)propyl)succinamide (DAPS), which demonstrated exceptional anticancer activity against human colon carcinoma cells (HT-29), highlighting its potential as a promising candidate for future anticancer therapies, supported by comprehensive evaluations including docking, molecular dynamics simulations, pharmacokinetic predictions, and ELISA assays.* ***Chapter V*** *describes a newly synthesized copper-based complex [Cu2L2(OAc)4] with 2-(3-(dimethylamino)propyl)isoindoline-1,3-dione as a ligand that exhibits dual enzymatic activities, acting as a catechol oxidase and phenoxazinone synthase under aerobic conditions, supported by various analyses, while also demonstrating significant anti-leukemic and anti-bacterial properties, making it a versatile bioinspired metallocatalyst with potential therapeutic applications. In C****hapter VI****, a novel copper-based metallocatalyst [Cu(L1)2(L2)] featuring P-hydroxybenzoic acid and N1,N1-dimethylpropane-1,3-*

diamine ligands that exhibits unique catechol oxidase and phenoxazinone synthase activities, characterized by distorted geometry, intricate molecular interactions, and oxygen-dependent enzymatic radical pathways, with exceptionally high catalytic efficiency and the generation of hydrogen peroxide as a key mechanistic feature. ***Chapter VII*** *includes future research in polydentate ligand-based metal complexes aiming to enhance oxidase activity that has the potential to yield novel multifunctional complexes with diverse applications in biotechnology, medicine, energy conversion, and industry, driving innovation across multiple disciplines.*

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It will be very difficult for me to mention each and every one and their contribution in this research work, but I want to take this opportunity to express my appreciation to a few who played a key role.

At first, on top for all, I owe many thanks to the almighty Allah for his protection and guidance in all aspects of my life.

Next, I would like to express my sincere thanks and gratitude to my research supervisor ***Dr. Rajesh Kumar Das*** *for his able guidance, valuable ideas, comments, expert teaching skill, valuable time, and tireless effort in supporting and supervising me. I would like to convey my sincere gratitude to* ***Prof. Somobrata Acharya***, School of Applied & Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Jadavpur, for XRD facility.

I am very much obliged to University of North Bengal for giving me the opportunity to pursue Ph. D. and all Staffs of the University of North Bengal for various official supports during the research work.

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Sahin Reja

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