समर्पण

आमा अनि बाबालाई

Dedicated to

My

Beloved Parents

DECLARATION

I declare that the thesis entitled "**ASSORTED INTERACTIONS OF SOME ANTIBACTERIAL AND ANTICANCER DRUG MOLECULES AND IONIC LIQUIDS PREVALING IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY INVESTIGATED BY EXPERIMENTAL AND COMPUTATIONAL APPROACH**" has been prepared by me under the guidance of Dr. Mahendra Nath Roy, Professor of Chemistry, University of North Bengal. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

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I certify that Ms Antara Sharma has prepared this thesis entitled "**ASSORTED INTERACTIONS OF SOME ANTIBACTERIAL AND ANTICANCER DRUG MOLECULES AND IONIC LIQUIDS PREVALING IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY INVESTIGATED BY EXPERIMENTAL AND COMPUTATIONAL APPROACH**" for the award of the Ph.D. degree from University of North Bengal under my supervision. She has carried out the work at the Department of Chemistry, University of North Bengal.

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ASSORTED INTERACTIONS OF SOME ANTIBACTERIAL AND ANTICANCER DRUG MOLECULES AND IONIC LIQUIDS PREVALING IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY INVESTIGATED BY EXPERIMENTAL AND COMPUTATIONAL APPROACH A thesis submitted to the UNIVERSITY OF NORTH BENGAL For the award of DOCTOR OF PHILOSOPHY (Ph.D.) In CHEMISTRY By ANTARA SHARMA, M.Sc. in Chemistry Supervisor DR. MAHENDRA NATH ROY, FRSC (London) Professor, Department of Chemistry University of North Bengal Darjeeling-734013, WB, INDIA June-2023

CHAPTER I NECESSITY OF THE RESEARCH WORK I.1. Objective, Scope and Applications of the Research work We live in a quickly growing and transient world with a numerous possibility. Gradual growth in technology, science makes greater impact in our society. Growth in scientific research led to many changes to traditional belief, systems, structures and mode of working thus exciting advanced opportunities are arising. These developments are leading to the change in the world of chemistry as a discipline and the role which chemists play. The environment where we work also changing. Scientific research helps to accumulate information and investigates different phenomena which in turn supports us to develop various theories and finally to understand nature. The gradual development in scientific research makes prediction-solving problems. Continuous involvement in research may create surprising outcomes. They may have direct impact in the immediate environment, such as related to chemical processes, or their developments in much broader context. Research creates new knowledge and understanding, thus helping us to plan the future to transform to the world of promising prospects. Understanding how existing trends in research have developed can help us to progress towards new paradigm of many unexplored fields in the future. Hence, scientific research is the key to realise everything that we have been doing, where we live, this earth and most importantly the whole universe. We human beings are doing research from centuries and science has reached to this stage through gradual contribution made by numerous scientist and researchers across the globe. This world is made up of molecules and interaction among variety of molecules such as living or non-living is the reason for our existence. As a result, a great deal of chemical research is dedicated to exploring matter – living organism interactions. These interactions can be of several types but the most important that we observe in living world is either

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I express my huge debt that I owe to the sources of information used for my research work - the various books, monographs, articles, websites, etc. I also extend my deep sense of gratitude to authors of all the publications I have cited in this thesis.

I acknowledge all my teachers who taught and inspired me in the various stages of life. The knowledge and motivation I have received from them has immensely inspired me in my research work.

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PREFACE

The research work described in this thesis entitled "**"ASSORTED NTERACTIONS OF SOME ANTIBACTERIAL AND ANTICANCER DRUG MOLECULES AND IONIC LIQUIDS PREVALING IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY INVESTIGATED BY EXPERIMENTAL AND COMPUTATIONAL APPROACH"** was started in January 2020 under the supervision of Prof. Mahendra Nath Roy, in Department of Chemistry, University of North Bengal.

The research work explores the supramolecular host – guest inclusion complex formation of some anticancer and antibacterial drug molecules as well as few biologically potent molecules with privileged structure, either to enhance or retain their biocompatibility by minimizing toxicity and also to develop the drug delivery system for feebly water soluble or insoluble molecules utilising highly sophisticated technique such as calorimetric, spectroscopic and various physiochemical methods. In addition to this biological activity, photo stability, thermal stability and solubility also investigated for these compounds. Therefore, simultaneously transforming these molecules into highly efficient drug in the form of inclusion complexes which leads the sustained release of the drug molecules to the target site without any chemical modification of the drug molecules. This thesis also includes the study of solute-solvent interaction between amino acid and ionic liquids to understand and evaluate the molecular interactions between ionic liquid and various biomolecules and also to interpret the behaviour of amino acid in complex structures of proteins.

In the journey of my research work, I am fortunate to participate in several seminars/conferences across the country. I was greatly influenced and motivated interacting with distinguished researchers and scientists, which immensely helped me in research through various way. I am very happy to publish my research work included in this thesis in the various journal of international repute.

In keeping with general practice of reporting scientific observation, due acknowledgement has been made whenever my work described in the thesis was inspired by the findings of other investigators. I must take the responsibility of any unintentional oversights and errors, which might have crept in spite of insurances.

I hope and expect challenges in my life to exercise my earned knowledge for the betterment and benefit of the society.

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	Figure 4: (B). SEM Image(a) IC1 NTF-α-CD Complex (b) NTF (c) α-CD (d) Physical mixture. **Figure: 5** (a) NFT-α-CD; side view (b) NFT-α-CD; upper view (c) NFT-β-CD; side view (d) NFT-β-CD; upper view**.** **Figure 6 :** (a) Comparative study of photostability of NTF, IC1 (NTF-β-CD) and IC1 (NTF-α-CD) (b) UV-visible spectra of pure NTF before and after exposure with sunlight (c) UV-visible spectra of Inclusion complex IC1 (NTF-β-CD) before and after exposure with sunlight, (d) UV-visible spectra of Inclusion complexIC2 (NTF-α-CD) before and after exposure with UV-light. **Figure.7:** Dose-dependent growth inhibition of human kidney cancer cell line (ACHN) after exposing with NTF, IC1 NTF-β-CD complex and IC2 NTF-α-CD complex for 48 h. **Figure 8:** UV-visible spectra of CT-DNA at different concentrations of a) NTF, b) IC2 (NTF-α-CD), c) IC1(NTF-β-CD) d) Comparison of CT-DNA interaction with NTF, IC2 (NTF-α-CD) and IC1(NTF-β-CD). **FigureS1:** Benesi-Hildebrand double reciprocal plot for the effect of β-CD on the absorbance of NTF (λ_{max} = 367 nm) at 298.15 K. **FigureS2:** Benesi-Hildebrand double reciprocal plot for the effect of α-CD on the absorbance of NTF (λ_{max} = 367 nm) at 298.15 K. **Figure S3:** ^{1}H-NMR spectra of β-CD, NTF and NTF-β-CD complex in DMSO-d_6 at 298.15K. **Figure S4:** ^{1}H-NMR spectra of α-CD, NTF and NTF-α-CD complex in DMSO-d_6 at 298.15K.	

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Chapter IV	**Scheme 1:** Molecular structures of (a) α-CD and (b) RH (c) β-CD (d) Cylindrical view of CDs. **Scheme 2:** Inclusion complex formation of Rhodanine with Cyclodextrin. **Scheme 3:** Table of Content.	119
Chapter V	**Scheme 1:** Molecular structures of (a) β-CD and (b) GEM(c) Cylindrical view of β-CD. **Scheme 2:** Inclusion complex formation of GEM with β-Cyclodextrin. **Scheme 3:** Table of Content.	154-155
Chapter VI	**Scheme1:** Structures of L-Leucine, benzyltriethylammonium chloride (BTEACl) and Benzyltributylammonium chloride (BTBACl). **Scheme 2:** Plausible molecular interactions between L-Leucine and Ionic Liquids, Hydrophobic-Hydrophobic interaction Ion-Hydrophobic Interaction Ion-Ion interaction.	205
Chapter VII	**Scheme 1:** Molecular structures of (a) α-CD and (b) β-CD (c) NTF (d) Cylindrical view of CDs. **Scheme 2:** Inclusion complex formation of Nitrofurantoin with Cyclodextrin. **Scheme 3:** Table of Content.	241

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APPENDIX A

LIST OF PUBLICATIONS

1. **Molecular assembly of rhodanine with torus shaped cyclodextrin and their innovative applications by physiochemical contrivance simultaneously optimized by computational study**

Chemistry Select, 2023, 8 (11), e202300417
(Included in the Thesis)

2. **Molecular encapsulation study of indole-3-methanol in cyclodextrins : Effect on antimicrobial activity and cytotoxicity**

Journal of Molecular Structure, 1225 (2021) 129093

3. **Physicochemical and computational investigations of some food chemicals prevalent in aqueous 1-butyl-1-methyl-pyrrolidinium chloride solutions with the manifestation of solvation consequences**

Journal of Molecular Liquids, 353 (2022) 118800

4. **Exploring inclusion complex of an anticancer drug with beta—cyclodextrin for reducing cytotoxicity towards normal human cell line by experimental and computational approach.**

Communicated to *ACS Omega* and it is under final revision

APPENDIX B

LIST OF SEMINARS/CONFERENCES ATTENDED

Sl. No.	Seminar/Conference	Date/Year	Organizer and Venue	Role
(1)	National Conference on "Environmental Determinism, Diverse Pollutions, Sources, and Controlling Management through Sciences and Humanities"	March 22-23, 2021	Alipurduar University	Oral Presentation
(2)	International Conference on Advances in Plants, Microbes and Agricultural Sciences	March 02-04, 2023	DBT, DST- SERB & Department of Botany, University of North Bengal	Oral Presentation
(3)	International Seminar on Frontiers in Chemistry 2023 & Prof. C. N. R. Rao Endowment Lecture	March 13-15, 2023	Department of Chemistry, University of North Bengal & CRSI North Bengal Local Chapter	Oral Presentation
(4)	National Science Day-2023"Global Science for Global Wellbeing"	February 28th 2023	Institution's Innovation Council (IIC), University of North Bengal	Poster Presentation