This thesis is

Dedicated to my

Beloved Parents,

Sister

And

My Respected Supervisors

For Their Constant Inspiration, Whole Hearted

Cooperation and Proper Valuable Guidance

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CERTIFICATE

I declare that **Ms. Debadrita Roy** has prepared the thesis entitled "**Investigation of Divergent Interactions of Some Noteworthy Compounds Prevalent in Host Guest and Solution Chemistry for Enhancing Applicability by Assorted Methodologies**" for the award of Ph. D degree of University of North Bengal under our joint guidance. She has carried out the work at the Department of Chemistry, University of North Bengal.

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DECLARATION

I declare that the thesis entitled **"Investigation of Divergent Interactions of some Noteworthy Compounds Prevalent in Host Guest and Solution Chemistry for Enhancing Applicability by Assorted Methodologies"** has been prepared by me for the Degree of Doctor of Philosophy (Ph.D) under the supervision of Prof. (Dr.) Biswajit Sinha, Professor of Chemistry, University of North Bengal and co-supervision of Dr. Subhadeep Saha (W.B.E.S.), Assistant Professor, Department of Chemistry, Government General Degree College at Pedong, Kalimpong – 734311, India. No part of the thesis has formed the basis for the award of any degree or fellowship previously, in this or any other Institution or University.

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Determination is a crucial prerequisite for accomplishing a goal, which can potentially be performed successfully through proper direction. At this time, I'd like to express my heartfelt gratitude to my respected supervisor, Dr. Biswajit Sinha, Professor, Department of Chemistry, University of North Bengal, West Bengal, India, and my respected co-supervisor, Dr. Subhadeep Saha (W.B.E.S.), Assistant Professor, Department of Chemistry, Government General Degree College at Pedong, Kalimpong - 734311, India. Throughout this challenging path, I have received continual counsel, useful suggestions, motivation, and inspiration from them. They deserve special recognition for not only providing me with his kind direction, but also motivating and encouraging me to go the extra mile along this journey. Without their care and assistance, I would not have been able to complete the thesis in its current shape. I am fortunate to have the opportunity to work under their supervision and would like to express my heartfelt gratitude to them.

I'd also like to thank all of the faculty members at the University of North Bengal's Department of Chemistry for their ongoing enthusiasm and inspiration during my research. I am also grateful to the university authorities, particularly the University Scientific Instrumentation Centre at the University of North Bengal, for providing me the laboratory resources for the study detailed in my thesis.

I specially thank all my lab-mates with whom I worked for their friendly help and encouragement throughout the present investigation.

My gratitude also extends to the sources of the information needed for my research: the countless books, monographs, articles, computer website, etc. I'd want to express my gratitude to individuals whose references I cited in this thesis.

I have to give credit to the people who helped me with this assignment; without their unwavering commitment and collaboration, I could not have finished it. I am deeply grateful to my mother, Smt. Madhabi Roy Isore, father, Dr. Mahendra Nath Roy, and sister, Smt. Madhusree Roy, for their unwavering support throughout these difficult circumstances. All that I am and will become in the future is a result of their immense blessings, dedication to my goals, and selflessness.

Finally, I would like to acknowledge my Respectable Grandfather, Grandmother, Uncle, Aunt and my Dearest Brother and Sister for their boundless and irreparable blessings, inspirations and wishes intending to augment the accomplishment of my Research Work associated with my PhD Thesis.

At last, I would like to thank all my well-wishers and many great people who helped and supported me directly or indirectly throughout this journey.

Debadrita Roy - 23/04/2024

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PREFACE

The research work of my thesis entitled "**Investigation of Divergent Interactions of some Noteworthy Compounds Prevalent in Host Guest and Solution Chemistry for Enhancing Applicability by Assorted Methodologies"** was initiated under the supervision of Dr. Biswajit Sinha, Professor, Department of Chemistry, University of North Bengal, West Bengal, India and co-supervision of Dr. Subhadeep Saha (W.B.E.S.), Assistant Professor, Department of Chemistry, Government General Degree College at Pedong, Kalimpong – 734311, India.

This work deals with the molecular inclusion complexes of cyclic host, oligosaccharide cyclodextrins with various guests like, drug molecules in solid and aqueous environments by various highly sophisticated spectroscopic techniques and physicochemical methods. I also investigated interactions of ionic liquids with bio-active molecules in the solution phase.

During my research work, I have participated in several workshops, conferences and seminars across the country and presented my research work. I was highly inspired by listening and interacting with renowned researchers, experts, reviewers and scientists which helped me a lot in my research work. I was even fortunate enough to publish the works in the thesis in International Journals of repute.

In observance with general practice of reporting scientific observation, due acknowledgement has been made whenever the work described was based on the finding of other investigators. I must take the responsibility of any unintentional omissions and errors, which might have crept in spite of insurances.

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LIST OF SCHEMES

ABBREVIATIONS

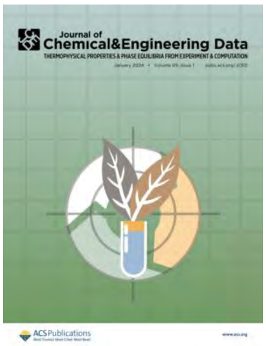
CD	Cyclodextrin
α-CD	α-cyclodextrin
HP-β-CD	2-Hydroxypropyl-β-cyclodextrin
IC	Inclusion complex
BNZ	Benserazide hydrochloride
ADP	Adiphenine hydrochloride
DPAH	D-Pantothenic acid hemicalcium salt
BTBAC	Benzyltributylammonium chloride
BTEAC	Benzyltriethylammonium chloride
BTMAC	Benzyltrimethylammonium chloride
L-Asparagine	L-Asp
TZ	Tartrazine
IL	Ionic liquid
AA	Amino acid
µm	Micrometre
Å	Angstrom
C	Carbon
H	Hydrogen
O	Oxygen
cm	Centimetre
DMF	Dimethylformamide
DMSO	Dimethyl sulfoxide
EtOH	Ethanol
Eq.	Equation
eV	Electron Volt
Fig.	Figure
ESI-MS	Electron Ionization Spray- Mass Spectrometry
g	Gram
hrs	Hours
Hz	Hertz
FTIR	Fourier Transform Infrared spectroscopy
K	Kelvin

M	Molar
m	Meter
mg	Milligram
min	Minute
mL	Millilitre
μM	Micromolar
μL	Microlitre
NIR	Near Infrared
^oC	Degree Celsius
pH	Potential of Hydrogen
rpm	Revolutions Per Minute
SEM	Scanning Electron Microscopy
TGA	Thermogravimetric Analysis
DSC	Differential Scanning Calorimetry
UV-vis	Ultraviolet-visible
NMR	Nuclear Magnetic Resonance
XRD	X-Ray Diffraction

APPENDIX A

LIST OF PUBLICATIONS

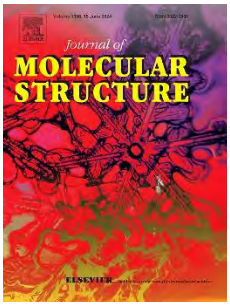
1. Exploration of Solvation Consequences of Ionic Liquids Prevalent in the Aqueous Media of Food Additive Azo Dye Tartrazine by Physicochemical and Computational Studies



J. Chem. Eng. Data **2024, 69, 1, 38–58**

(Included in the Thesis)

2. Probing supramolecular complexation of the drug benserazide hydrochloride with hydroxypropyl-β-cyclodextrin by experimental and computational studies



Journal of Molecular Structure, (1294) Part 1, 2023, 136329

(Included in the Thesis)

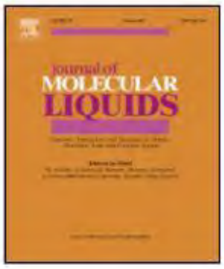
3. Physicochemical investigation of L-Asparagine in green solvent arrangements with the manifestation of solvation consequences

WJARR

World Journal of Advanced Research and Reviews, 2022, 13(02), 401–428

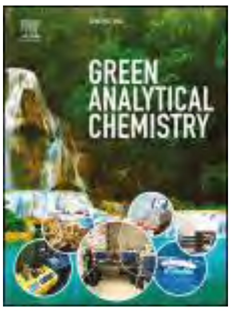
(Included in the Thesis)

4. Exploring 2:1 inclusion complexes of cyclodextrins and antispasmodics, Alverine citrate for enhancing bioavailability and sustained dischargement



Journal of Molecular Liquids, (370), 2023, 121036

5. A green approach towards the removal of a water pollutant by encapsulation of HBCDD into cyclodextrins: Combined experimental and theoretical studies

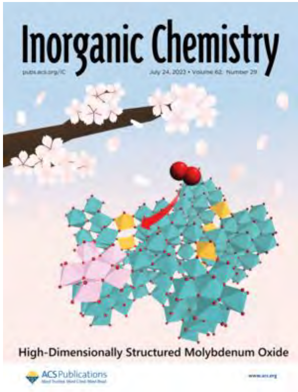


Green Analytical Chemistry,(8), 2024, 100097

6. Synthesis, crystal structure, Hirshfeld surface, and DFT studies of a Copper(II) complex of 5,5′-dimethyl-2,2′-bipyridine and 1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid

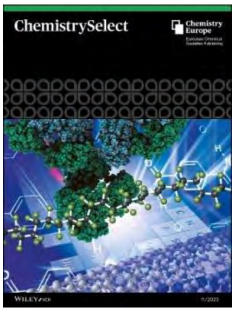
Results in Chemistry,(6), 2023, 101050

7. Label-Free Detection of Epinephrine Using Flower-like Biomimetic CuS Antioxidant Nanozymes



***Inorg. Chem.* 2023, 62, 29, 11291–11303**

8. Molecular Assembly of Rhodanine with Torus-Shaped Cyclodextrins and Their Innovative Applications by Physicochemical Contrivance Simultaneously Optimized by Computational Study



Chem Select, 8, 11,2023,e202300417

9. Fe–Mn nanocomposites doped graphene quantum dots alleviate salt stress of *Triticum aestivum* through osmolyte accumulation and antioxidant defense

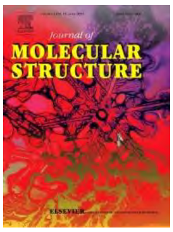
Scientific Reports

Scientific Reports **volume 13, Article number: 11040 (2023)**

10. Inclusion of an antiplatelet agent inside into β-cyclodextrin for biochemical applications with diverse authentications

Food Chemistry Advances, Volume 1, October 2022, 100015

11.Encapsulated hydroxychloroquine and chloroquine into cyclic oligosaccharides are the potential therapeutics for COVID-19: insights from first-principles calculations



Journal of Molecular Structure,Volume 1247, 5 January 2022, 131371

List of Seminars/Symposiums/Conferences Attended

- DBT & DST-SERB (Govt. of India) Sponsored International Conference on " Advances in Plants, Microbes and Agricultural Sciences", Organised by DST (FIST) & UGC-SAP assisted DRS, Department of Botany, University of North Bengal, 2nd –4th March, 2023. **(*Best Oral Presentation)***

- International Seminar on Frontiers in Chemistry 2023 & Prof. C. N. R. Rao Endowment Lecture, Department of Chemistry, University of North Bengal, 13-15th March, 2023. (***Presented a Poster***)

- National Conference on " Environmental Determinism, Diverse Pollutions, Sources, And Controlling Management Through Sciences and Humanities", Organized by Alipurduar University, 22nd and 23rd March, 2021. ***(Presented a Paper)***

- Annual Convention of Chemists and International Conference on Recent Trends in Chemical Sciences, 21st – 24th December,2021.***(Participation)***

- SERB Sponsored KARYASHALA, on a Hands-on training Program on Design, synthesis, characterization and understanding of smart functional materials through experimental and computational modelings, by Dept. of Chemistry, University of North Bengal, Darjeeling, (04th July– 11th July, 2022), ***(Participation)***

- Science Academies Lecture Workshop on " New Facets in Chemical Sciences: Challenges and Opportunities" from 22-23rd March 2024 organized by the Department of Chemistry, University of North Bengal, Darjeeling 734013. ***(Participation)***