THIS THESIS IS

DEDICATED TO MY

BELOVED PARENTS, FREEDOM FIGHTER

GRANDFATHER, GRANDMOTHER,

BROTHER

AND

MY RESPECTED SUPERVISORS

FOR THEIR CONSTANT INSPIRATION, WHOLE HEARTED COOPERATION AND PROPER VALUABLE GUIDANCE

Ouriginal

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I, certify that Mr. Biswajit Ghosh has prepared his thesis entitled *"PHYSICOCHEMICAL STUDIES OF DIVERSE INTERACTIONS OF SOME SELECTED SIGNIFICANT MOLECULES PREVALENT IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY"*, for the award of **Ph. D. degree (Doctor of Philosophy)** from the University of North Bengal, under our guidance. He has carried out his work at the Department of Chemistry, University of North Bengal. The contents of this thesis, in full or in parts, have not been submitted to any other Institution or University for the award of any degree or diploma.

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DECLARATION

I declare that the thesis entitled *"PHYSICOCHEMICAL STUDIES OF DIVERSE INTERACTIONS OF SOME SELECTED SIGNIFICANT MOLECULES PREVALENT IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY"* has been prepared by me for the degree of **Doctor of Philosophy (Ph.D.)** under the supervision of **Dr. Mahendra Nath Roy, FRSC (London), (Principal Supervisor)**, Professor of Chemistry, University of North Bengal and Dr. Vikas Kumar Dakua (Co-Supervisor), Asst. Professor of Chemistry, Alipurduar University. No part of this thesis has formed the basis for the award of any other degree or diploma, in this or any other Institution or University.

Biswajit Ghosh (17-04-2023)

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ACKNOWLEDGEMENT

First and foremost, praises and thanks to the Almighty God for his blessings throughout my research work to complete my research successfully.

First of all, I would like to convey my most deep sense of gratitude to my respected supervisor, ***Dr. Mahendra Nath Roy, FRSC (London)***, Professor of Chemistry, University of North Bengal, West Bengal, India. Throughout my research phase, I have received constant supervision, valuable suggestions and inspiration from him in every possible way. I feel blessed and privileged to finish my thesis under his guidance, who trusted me completely and gave independence to explore different ideas of my own. Without his continuous encouragement, responsible guidance, and priceless supervision, the research work associated with this thesis would not have been possible.

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I express my special thanks to the editors, co-editors and reviewers of my publications as the comments and suggestions from them have also been valuable for carrying out the research works. All the cited references are the major sources of information which helps us to develop new ideas, and hence, all the authors/ researchers behind the cited works are hereby sincerely thanked.

I must acknowledge all my respected teachers who taught me in Changrabandha Higher Secondary School, Ananda Chandra College, Jalpaiguri, and University of North Bengal. The knowledge I received from them has really helped me to carry out my research work.

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PREFACE

The research work in the thesis entitled ***"PHYSICOCHEMICAL STUDIES OF DIVERSE INTERACTIONS OF SOME SELECTED SIGNIFICANT MOLECULES PREVALENT IN SUPRAMOLECULAR AND SOLUTION CHEMISTRY"*** was initiated under the supervision of ***Dr. Mahendra Nath Roy,*** **FRSC (London)**, **(Principal Supervisor)**, Professor of Chemistry, University of North Bengal and Dr. Vikas Kumar Dakua (Co-Supervisor), Asst. Professor of Chemistry, Alipurduar University.

The whole work is an attempt to explore the supramolecular *"Host–Guest"* inclusion complexation of some biologically active molecules such as small drug molecules, vitamins, in order to make them more bioavailable by increasing their solubility and controlled release without any chemical modification of the bioactive molecules. Beside this, we investigated molecular interactions between amino acid- ionic liquid in aqueous medium by studying their thermodynamic and transport properties.

During the course of my research, I was privileged to participate in several meets and seminars across the country. I was highly inspired by listening and interacting with distinguished experts and scientists. I was very fortunate enough to publish my research works relating the thesis in the International Journal of repute.

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

I hope I will be given more challenges in my life so that the knowledge that I have earned during my work can be put into action in the future.

LIST OF TABLES

LIST OF FIGURES

LIST OF SCHEMES

ABBREVIATIONS

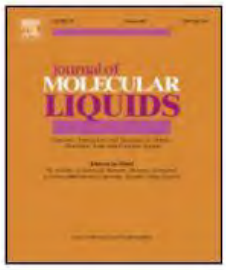
CD	Cyclodextrin
αCD	α-cyclodextrin
βCD	β-cyclodextrin
TSC4X	p-sulfonatothiacalix[4]arene
IC	Inclusion complex
MEP	Mephenesin
PTU	6-propyl-2-thiouracil
NB	Nile blue
BTBACl	Benzyltributylammonium chloride
RIBO	Riboflavin
IL	Ionic liquid
AA	Amino acid
BSA	Bovine Serum Albumin
CT-DNA	Calf Thymus DNA
DPPH	2,2-Diphenyl-1-Picrylhydrazyl
DPBF	1,3-Diphenylisobenzofuran
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
^{0}C	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

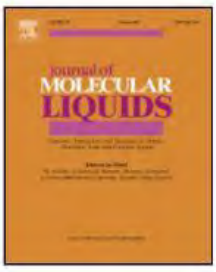
1. **B. Ghosh,** N. Roy, D. Roy, S. Mandal, S. Ali, P. Bomzan, K. Roy and M. N. Roy, An extensive investigation on supramolecular assembly of a drug (MEP) with βCD for innovative applications.



Journal of Molecular Liquids, 344, (2021) 117977

(Included in the Thesis)

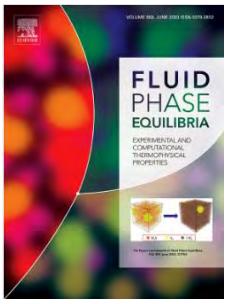
2. **B. Ghosh,** N. Roy, D. Roy, S. Mandal, M. Mondal, V. K. Dakua, A. Dutta, S. Sen, A. Kumar, R. Chakraborty and M. N. Roy, Exploring inclusion complex of an antithyroid drug (PTU) with α-Cyclodextrin for innovative applications by physicochemical approach optimized by molecular docking.



Journal of Molecular Liquids, 380, (2023) 121708

(Included in the Thesis)

3. **B. Ghosh,** A. Sinha, N. Roy, B. Rajbanshi, M. Mondal, D. Roy, A. Das, N. N. Ghosh, V. K. Dakua and M. N. Roy, Molecular interactions of some bioactive molecules prevalent in aqueous ionic liquid solutions at different temperatures investigated by experimental and computational contrivance.



Fluid Phase Equilibria, 557, (2022) 113415

(Included in the Thesis)

4. **B. Ghosh,** N. Roy, S. Mandal, S. Ali, P. Bomzan, D. Roy, M. Salman Haydar, V. K. Dakua, A. Upadhyay, D. Biswas, K. K. Paul and M. N. Roy, Host–Guest Encapsulation of RIBO with

TSC4X: Synthesis, Characterization, and Its Application by Physicochemical and Computational Investigations.

ACS Omega, 8, 7, (2023) 6778-6790

(Included in the Thesis)

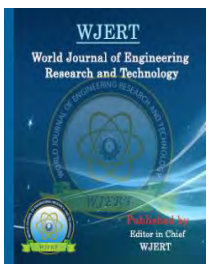
5. N. Roy, P. Bomzan, **B. Ghosh** and M. N. Roy, A Combined Experimental and Theoretical Study on p-Sulfonatothiacalix [4] arene Encapsulated Sulisobenzone.

New Journal of Chemistry, 47, (2023) 1045-1049

6. M. Mondal, S. Basak, S. Ali, D. Roy, S. Saha, **B. Ghosh,** N. N. Ghosh, K. Lepcha, K. Roy and M. N. Roy, Exploring inclusion complex of an anti-cancer drug (6-MP) with β-cyclodextrin and its binding with CT-DNA for innovative applications in anti-bacterial activity and photostability optimized by computational study.

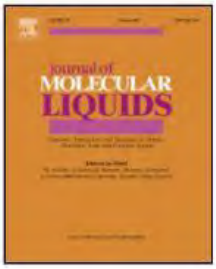
RSC Advances, 12, 48, (2022) 30936-30951

7. B. Saha, S. Barman, S. Majumder, N. Roy, **B. Ghosh,** R. Chakrabarty, S. Choudhury, N. N. Ghosh, K. Baul and M. N. Roy, Physicochemical studies of biologically potent molecules in aqueous ionic liquid solutions with the manifestation of solvation consequences at different temperatures optimized by computational investigations.



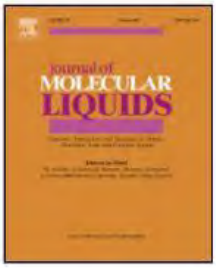
World Journal of Engineering Research and Technology, 8,10, (2022) 44-89

8. N. Roy, P. Bomzan, D. Roy, **B. Ghosh** and M. N. Roy, Exploring β-CD grafted GO nanocomposites with an encapsulated fluorescent dye duly optimized by molecular docking for better applications.



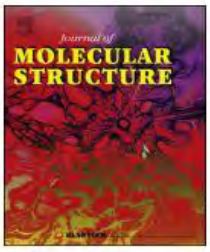
Journal of Molecular Liquids, 329, (2021) 115481

9. M. Mondal, S. Basak, **B. Ghosh,** S. Ali, B. Saha, K. Mallick, K. Roy and M. N. Roy, A Combined Physicochemical and Computational Investigation of the Inclusion Behaviour of 3-(1-Naphthyl)-D-alanine Hydrochloride insights into β-Cyclodextrin.



Journal of Molecular Liquids, 378, (2023) 121583

10. P. Bomzan, N. Roy, **B. Ghosh** and M. N. Roy, Exploring inclusion complexes of amino acids with *p*-sulfonatothiacalix[4]arene by experimental and computational approach.

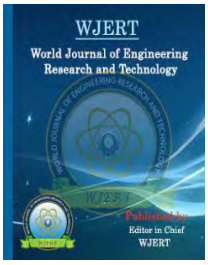


Journal of Molecular Structure, 1231 (2023) 133982

11. M. Mondal, S. Basak, D. Roy, M. S. Haydar, S. Choudhury, **B. Ghosh,** N. N. Ghosh, A. Dutta, P. Mandal, K. Roy, A. Kumar and M. N. Roy, Probing the molecular assembly of a metabolizer drug with β-cyclodextrin and its binding with CT-DNA in augmenting antibacterial activity and photostability by physicochemical and computational methodologies.

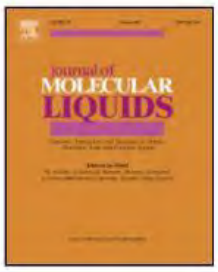
ACS Omega, 7, 30, (2022) 26211-26225

12. S. Debnath, A. Poddar, A. Sinha, A. Hossain, **B. Ghosh,** S. Majumder, M. Mondal, N. Roy, B. Rajbanshi and M. N. Roy, Physicochemical investigation of diverse interactions of some biologically potent molecules in aqueous green environments at different temperatures.



World Journal of Engineering Research and Technology, 8, 10, (2021) 90-111

13. M. Mondal, S. Basak, D. Roy, S. Saha, **B. Ghosh,** S. Ali, N. N. Ghosh, A. Dutta, A. Kumar and M. N. Roy, Cyclic oligosaccharides as controlled release complexes with food additives (TZ) for reducing hazardous effects.



Journal of Molecular Liquids, 348, (2022) 118429

14. S. Majumder, A. Sinha, D. Roy, **B. Ghosh,** N. N. Ghosh, T. Roy, V. K. Dakua, A. Datta, I. Sarkar, S. Choudhury, A. Roy, N. Roy and M. N. Roy, Exploration of Diverse Interactions of l -Methionine in Aqueous Ionic Liquid Solutions: Insights from Experimental and Theoretical Studies.

ACS Omega, 2c08008 (2023)

15. N. Roy, **B. Ghosh,** D. Roy, B. Bhaumik and M. N. Roy, Exploring the inclusion complex of a drug (umbelliferone) with α-cyclodextrin optimized by molecular docking and increasing bioavailability with minimizing the doses in human body.

ACS Omega, 5, 46, (2020) 30243-30251

APPENDIX-B

LIST OF SEMINARS/CONFERENCES ATTENDED

1. National Seminar on "Frontiers in Chemistry – **2020**" Organised by: Department of Chemistry, University of North Bengal & CRSI North Bengal Local Chapter, March 5, 2020. ***(Presented a poster)***

2. National Web-Based Conference on "Environmental Determinism, Diverse Pollutions, Sources, and Controlling Management Through Sciences and Humanities" Organised by: Alipurduar University, 22nd and 23rd March, 2021. ***(Presented a paper)***

3. International Web-Based Conference on "Emerging Issues of the New SARS COV-2 variant Omicron and Its Impact on Society, Economy and Culture" Organised by: Alipurduar University, 28th February and 1st March, 2022. ***(Presented a paper)***

4. International Seminar on "Frontiers in Chemistry **2023**" Organised by: Department of Chemistry, University of North Bengal & CRSI North Bengal Local Chapter.