

***This Thesis is dedicated
to
my beloved
Parents, Brother,
Grandparents, Husband and
my Supervisor.***

For Their Constant Inspiration, Whole Hearted
cooperation and Proper valuable guidance



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Submission Information

Author Name	Baishali Saha
Title	Various Interactions Prevailing in Supramolecular Assembly and Different Liquid Systems Probed by Experimental and Theoretical Studies for Innovative Applications
Paper/Submission ID	1607041
Submitted by	nbuplg@nbu.ac.in
Submission Date	2024-04-05 11:28:58
Total Pages	247
Document type	Thesis

Result Information

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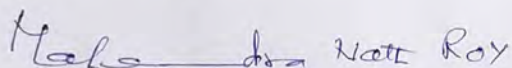
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CERTIFICATE

I, certify that Smt. Baishali Saha has prepared her thesis entitled **“Various Interactions Prevailing in Supramolecular Assembly and Different Liquid Systems Probed by Experimental and Theoretical Studies for Innovative Applications”**, for the award of **Ph.D. Degree (Doctor of Philosophy)** from the University of North Bengal, under my guidance. She has carried out her 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 "**Various Interactions Prevailing in Supramolecular Assembly and Different Liquid Systems Probed by Experimental and Theoretical Studies for Innovative Applications**" has been prepared by me for the degree of **Doctor of Philosophy (Ph.D.)** under the supervision of **Dr. Mahendra Nath Roy, FRSC (London), Supervisor**, Professor of Chemistry, University of North Bengal. 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.

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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.

My Special thanks to our *Hon'ble Head of department of chemistry, NBU*, Prof. (Dr.) **Bhaskar Biswas** for his continuous and comprehensive suggestion and guidance in the research work.

I also express my earnest gratitude to the honourable faculty members', officers and other academic staffs of Department of Chemistry, University of North Bengal for their helpful assistance and continual inspiration during the course of my research. I am grateful to the University authority for providing laboratory facilities, especially USIC, NBU for giving me instrumental facilities.

I would also like to extend my deepest appreciation to **Mr. Sanjoy Barman, Mr. Modhusudan Mondal, Dr. Subhankar Choudhury, Dr. Sukdev Majumder, Dr. Subhadeep Saha, Dr. Biswajit Ghosh** and all other labmates for their valuable assistance, suggestion and cooperation during my research work.

The people, without the whole hearted willingness and cooperation of whom I would not be able to complete this task must be acknowledged. I am extremely grateful to my beloved father, **Sri. Bikash Chandra Saha** and mother, **Smt. Nandita Saha**, for their unconditional love, care, prayers, and sacrifices for educating and preparing me for my future. Also, I would like to place my sincere gratitude to my grandfathers, **Late Sri. Naba Gopal Talukdar, Late Sri. Birendra Nath Saha**, grandmothers, **Smt. Tripti Rani Talukdar**, and **Late Smt. Basanti Rani Saha**, my beloved brothers **Mr. Bishal Saha, Mr. Sourik Talukdar**, and sister **Miss. Soyeta Majumder**, my maternal uncle, **Sri. Amit Talukdar**, maternal aunt, **Smt. Pinki Paul Talukdar**, aunt, **Smt. Sangita Majumder** for

their constant support and whole hearted cooperation with a view to augmenting the various work associated with my Ph.D. thesis during my research work. I thank them for their immense blessings and wishes to me all the time. Whatever I am today and whatever I will be in future is because of their enormous blessings and wishes, and commitments to my ambitions.

Special thanks to my beloved husband **Mr. Sanjoy Barman** for his constant love, care and motivation. I also extend my gratitude towards my father in law **Sri. Bhupesh Chandra Barman**, mother in law **Smt. Shampa Barman**, brother in law **Mr. Dhananjay Barman** and sister in law **Miss. Papiya Barman** and **Smt. Jaysree Barman Das**.

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 Maynaguri Girls' High School, Prasannadeb Women's College, Jalpaiguri, and University of North Bengal. The knowledge I received from them has really helped me to carry out my research work.

Finally, I would like to express my acknowledgement to the Swami Vivekananda Merit Cum Means Scholarship (SVMCM), reference number WBP211628595537 for financial support to continue this research work. University Grants Commissions' Special Assistance Programme Departmental Research Support-III (SAP-DRS-III) provides sophisticated instrumental facilities. I am also thankful to the 'ONE TIME GRANT' Ref No. F.4-10/2010(BSR) awarded to my Supervisor, Prof. (Dr.) Mahendra Nath Roy, under Basic Scientific Research (BSR), UGC, New Delhi for financial and instrumental assistance in connection with my research works.

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PREFACE

The research work in the thesis entitled **“Various Interactions Prevailing in Supramolecular Assembly and Different Liquid Systems Probed by Experimental and Theoretical Studies for Innovative Applications”** was initiated under the supervision of **Prof. (Dr.) Mahendra Nath Roy, FRSC (London), Supervisor**, Professor of Chemistry, University of North Bengal.

The whole work is an attempt to explore the supramolecular *“Host-Guest”* inclusion complexation of some biologically active molecules such as drug molecules, dye, in order to make them more bioavailable by increasing their photostability, cytotoxicity against cancer cell and controlled release without any chemical modification of the bioactive molecules. Beside this, we investigated molecular interactions between amino acid- ionic liquid, amino acid-drug 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

CHAPTERS	TABLES	PAGE NO.
CHAPTER IV	Table 1: Details of Chemical Name, Attribution, CAS Number and Mass Fraction of Materials Studied.	78
	Table 2: Apparent molar volume (ϕ_v^0), viscosity- <i>B</i> and viscosity- <i>A</i> coefficient and Molar Refraction (R_M^0) of (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous ionic liquid BTEAC solutions of different concentrations (molality) 0.001 m, 0.003 m, 0.005 m at temperatures 298.15 K, 303.15 K, 308.15 K, and 313.15 K.	78
	Table 3: Values of various coefficients of equation-5 for L-Alanine and L-Isoleucine in different molalities (<i>m</i>) of aqueous IL (BTEAC) solutions.	80
	Table 4: Values of limiting molar expansibilities ($\delta\phi_E^0 / \delta T$) _{<i>p</i>} for L-Alanine and L-Isoleucine in different concentration (molality) of aqueous IL (BTEAC) solutions at different temperatures.	80
	Table 5: Values of B/ϕ_v^0 for L-Alanine and L-Isoleucine in different concentrations (m) of aqueous IL (BTEAC) mixtures at four different temperatures.	80
	Table 6: dB/dT data of amino acids taken in the aqueous BTEAC solutions.	81
	Table 7: Values of $(\bar{V}_1^0 - \bar{V}_2^0)$, $\Delta\mu_1^{0\neq}$, $\Delta\mu_2^{0\neq}$, $T\Delta S_2^{0\neq}$, and $\Delta H_2^{0\neq}$ for L-Alanine and L-Isoleucine in different molality (<i>m</i>) of aqueous IL (BTEAC) solutions at various temperatures.	81
	Table 8: Limiting Slopes ($\partial\sigma/\partial m$) data of the surface tension of amino acids taken in the aqueous solutions.	82
	Table 9: ΔH° (Kcal); ΔG° (Kcal) and ΔS° (cal/K) for (a) L- Alanine + BTEAC (b) L-Isoleucine+ BTEAC complexes in water medium.	82
	Table S1: Density (ρ), Viscosity (η), Refractive index (n_D) of aqueous pure BTEAC solutions of concentrations (molality) 0.001 m, 0.003 m, 0.005 m at temperatures 298.15 K, 303.15 K, 308.15 K, and 313.15 K.	83
	Table S2: Density (ρ), Viscosity (η), Refractive index	83

LIST OF TABLES

CHAPTERS	TABLES	PAGE NO.
	(n_D) of aqueous pure (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality), 0.001 m at temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.	
	Table S3: Density (ρ), Viscosity (η), Refractive index (n_D) of aqueous pure (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality), 0.003 m at temperatures 298.15 K, 303.15 K, 308.15 K, and 313.15 K.	84
	Table S4: Density (ρ), Viscosity (η), Refractive index (n_D) of aqueous pure (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality), 0.005 m at temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.	85
	Table S5: Apparent molar volume (ϕ_V), $(\eta_r-1)/\sqrt{c}$ and Molar Refraction (R_M) of aqueous pure (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality), 0.001 m at temperatures 298.15 K, 303.15 K, 308.15 K, and 313.15 K.	86
	Table S6: Apparent molar volume (ϕ_V), $(\eta_r-1)/\sqrt{c}$ and Molar Refraction (R_M) of aqueous pure (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality), 0.003 m at temperatures 298.15 K, 303.15 K, 308.15 K, and 313.15 K.	87
	Table S7: Apparent molar volume (ϕ_V), $(\eta_r-1)/\sqrt{c}$ and Molar Refraction (R_M) of aqueous pure (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality) 0.005 m at temperatures 298.15 K, 303.15 K, 308.15 K, and 313.15 K.	88
	Table S8: Molar conductivities of (L-ALANINE + BTEAC + H ₂ O) and (L-ISOLEUCINE + BTEAC + H ₂ O) systems in aqueous BTEAC solutions of concentration (molality), 0.001 m, 0.003 m, 0.005 m at temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.	89

CHAPTERS	TABLES	PAGE NO.
	K.	
	Table S9: Surface Tension σ of L-Alanine and L-Isoleucine as a function of different concentration (molality) of aqueous BTEAC solutions at temperatures 298.15 K.	90
	Table S10: UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (L-Alanine+BTEAC) system at 298.15 K.	92
	Table S11: UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (L-Isoleucine+BTEAC) system at 298.15 K.	92
CHAPTER V	Table 1: Limiting apparent molar volume (ϕ_v^0), Regression Co-efficient (R^2), Experimental slope (S_v^*), Viscosity- B and Viscosity- A coefficient term, and Limiting molar Refraction (R_M^0) of (L-Val + aqueous MEPN) and (L-Phe + aqueous MEPN) systems of altered concentrations (molality) of MEPN in aqueous solution at changing temperatures.	124
	Table 2: Volume transfer/ $\Delta_{tr}\Phi_v^0$ for L-Val/L-Phe aqueous solutions of (0.001, 0.003, 0.005) mol.kg ⁻¹ MEPN at 298.15 K, 303.15 K, 308.15 K, 313.15 K at atmospheric pressure 0.1 mPa.	125
	Table 3: Values of $(\bar{V}_1^0 - \bar{V}_2^0)$, $\Delta\mu_1^{0\neq}$, $\Delta\mu_2^{0\neq}$, $T\Delta S_2^{0\neq}$, and $\Delta H_2^{0\neq}$ for L-Val and L-Phe in altered concentrations of MEPN in aqueous solution at changing temperatures.	126
	Table 4: Limiting Slopes ($\partial\sigma/\partial m$) of surface tension of AAs selected in the aqueous MEPN solutions.	127
	Table S1: Descriptions of Chemicals taken.	127
	Table S2: Density (ρ), Viscosity (η), and Refractive index (n_D) of pure aqueous MEPN solutions of concentrations (molality) 0.001 m , 0.003 m , 0.005 m at temperatures $T=298.15$ K, 303.15 K, 308.15 K, and 313.15 K.	128
	Table S3: Density (ρ), Viscosity (η), and Refractive index (n_D) of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in 0.001 molal of MEPN in	128

CHAPTERS	TABLES	PAGE NO.
	aqueous solutions at temperatures $T=298.15$ K, 303.15 K, 308.15 K, and 313.15 K.	
	Table S4: Density (ρ), Viscosity (η), and Refractive index (n_D) of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in 0.003 molal of MEPN in aqueous solutions at temperatures $T=298.15$ K, 303.15 K, 308.15 K, and 313.15 K.	129
	Table S5: Density (ρ), Viscosity (η), and Refractive index (n_D) of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in 0.005 molal of MEPN in aqueous solutions at temperatures $T=298.15$ K, 303.15 K, 308.15 K and 313.15 K.	130
	Table S6: Empirical Coefficients of equation-5 for L-Val and L-Phe in changed concentrations (molality) of MEPN in aqueous solution.	131
	Table S7. Limiting molar expansibility $(\delta\phi_E^0 / \delta T)_P$ terms for L-Val and L-Phe in altered concentrations (molality) of MEPN in aqueous solution at changing temperatures.	131
	Table S8: B/ϕ_V^0 terms for L-Val and L-Phe in changing concentrations (molality) of MEPN in aqueous solution at altered temperatures.	132
	Table S9: dB/dT outcomes of AAs observed in the aqueous MEPN solutions.	132
	Table S10: Apparent molar volume (ϕ_V), $(\eta_r-1)/\sqrt{c}$, and Molar Refraction (R_M) of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in 0.001 molal of MEPN in aqueous solutions at temperatures $T=298.15$ K, 303.15 K, 308.15 K and 313.15 K.	132
	Table S11: Apparent molar volume (ϕ_V), $(\eta_r-1)/\sqrt{c}$, and Molar Refraction (R_M) of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in 0.003 molal of MEPN in aqueous solutions at temperatures $T=298.15$ K, 303.15 K, 308.15 K, and 313.15 K.	133
	Table S12: Apparent molar volume (ϕ_V), $(\eta_r-1)/\sqrt{c}$ and Molar Refraction (R_M) of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in 0.005 molal of MEPN in aqueous solutions at temperatures $T=298.15$ K, 303.15 K, 308.15 K, and 313.15 K.	134

CHAPTERS	TABLES	PAGE NO.
	Table S13: Molar conductivities of (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in aqueous MEPN solutions of concentration 0.001 molal, 0.003 molal, 0.005 molal at temperatures $T=298.15$ K, 303.15 K, 308.15 K, and 313.15 K.	135
	Table S14: Surface Tension (σ) for both (L-Phe + aqueous MEPN) and (L-Val + aqueous MEPN) systems in altered concentrations of MEPN in aqueous solutions at temperature $T=298.15$ K.	136
	Table S15: UV-Vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (L-Val + aqueous MEPN) system at $T=298.15$ K.	137
	Table S16: UV-Vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (L-Phe + aqueous MEPN) system at $T=298.15$ K.	138
	Table S17: Density (ρ) of L-Valine and L-Phenylalanine in aqueous solutions at 298.15 K, 303.15 K, 308.15 K, and 313.15 K at atmospheric pressure 0.1 mPa.	138
	Table S18: Limiting apparent molar volumes (ϕ_V^θ), experimental slopes (S_V^*), of L-Val/L-Phe in aqueous solutions at various working temperatures and atmospheric pressure at 0.1 mPa.	138
	Table S19: Apparent molar volume, (V_ϕ) of L-Val /L-Phe in aqueous solution at different temperatures $T=(298.15 - 313.15)$ K at atmospheric pressure 0.1 mPa.	139
CHAPTER VI	Table 1: Chemical shifts data (in ppm) of various protons in the free state of BB and β -CD and its BBIC.	169
	Table 2: FTIR data of pure BB, β -CD, and BBIC complex.	169
	Table 3: The surface tension value at the breakpoint and the corresponding concentrations of BB and β -CD (mM) at 298.15 K.	170
	Table 4: The conductance value at the breakpoint and the corresponding concentrations of BB and β -CD (mM) at 298.15 K.	170
	Table 5: Values of association constant and Gibbs free energy change of the BB+ β -CD system from UV-visible spectroscopy.	170

LIST OF TABLES

CHAPTERS	TABLES	PAGE NO.
	Table 6: Values of the association constant and Gibbs free energy change of the BB+ β -CD system from fluorescence study.	171
	Table 7: Binding constant values of BB and BBIC with CT-DNA.	171
	Table 8: Adsorption energy; HOMO, LUMO levels, band gap, and other global parameters for BB and BB- β -CD inclusion complexes in water medium.	171
	Table S1: Data for the Job plot performed by UV-Vis spectroscopy for BB+ β -CD system at 298.15 K ^a .	172
	Table S2: Data for the surface tension study of BB+ β -CD system (concentration of stock solution of BB = 10mM, concentration of stock solution of β -CD = 10mM) at 298.15 K ^a .	172
	Table S3: Data for the conductivity study of BB+ β -CD system (concentration of stock solution of BB = 10mM, concentration of stock solution of β -CD = 10mM) at 298.15 K ^a .	173
	Table S4: Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for BB+ β -CD system.	173
	Table S5: Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for BB+ β -CD system with gradual addition of lower concentration of aqueous β -CD solutions.	174
	Table S6: Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for BB+ β -CD system with gradual addition of higher concentration of aqueous β -CD solutions.	174
	Table S7: Data for the Benesi-Hildebrand double reciprocal plot performed by Fluorescence spectroscopy for BB+ β -CD system.	175
	Table S8: Data for the Job plot performed by Fluorescence spectroscopy for BB+ β -CD system at 298.15 K ^a .	175
CHAPTER VII	Table 1: Composition of gel.	208
	Table 2: Chemical shifts data (in ppm) of various protons in the free state of VC and γ -CD and ICVC.	209

CHAPTERS	TABLES	PAGE NO.
	Table 3; The conductance value at the breakpoint and the corresponding concentrations of VC and γ -CD (mM) at 298.15 K.	209
	Table 4: The surface tension value at the break point and the corresponding concentrations of VC and γ -CD (mM) at 298.15 K.	209
	Table 5: Values of association constant and Gibbs free energy change of the VC+ γ -CD system from UV-visible spectroscopy.	210
	Table 6: Physicochemical characterization parameters of experimental VC and ICVC containing gel (n=3).	210
	Table 7: Different kinetic equations and R^2 values obtained from optimised formulation VL5 <i>in vitro</i> drug release kinetics.	210
	Table 8: Permeability Parameters of Different Formulations.	211
	Table S1: Data for the Job's plot performed by UV-Vis spectroscopy for VC+ γ -CD system at 298.15 K ^a .	211
	Table S2: Data for the conductivity study of VC+ γ -CD system (concentration of stock solution of VC = 10 mM, concentration of stock solution of γ -CD = 10 mM) at 298.15 K ^a .	211
	Table S3: Data for the surface tension study of VC+ γ -CD system (concentration of stock solution of VC = 10 mM, concentration of stock solution of γ -CD = 10 mM) at 298.15 K ^a .	212
	Table S4: Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for VC+ γ -CD system.	213

LIST OF FIGURES

CHAPTERS	TABLES	PAGE NO.
CHAPTER I	Figure 1: Schematic illustration of host-guest supramolecular inclusion complex.	2
CHAPTER II	Figure 1: Van der Waals forces acting between molecules.	15
	Figure 2: Hydrogen bonding in water molecules.	15
	Figure 3: Hydrophobic interaction brings the interacting molecules closer.	16
	Figure 4: Electrostatic force working between charged species.	17
	Figure 5: Dipole-Dipole attraction between the polar molecules.	18
	Figure 6: Ion-Dipolar attraction between the ion and polar molecules.	1
	Figure 7: Schematic representation of an NMR instrument.	20
	Figure 8: A schematic diagram of a Fourier Transform Infrared (FTIR) Spectrophotometer	21
	Figure 9: Schematic diagram of UV-visible spectrophotometer.	23
	Figure 10: Jablonski Diagram.	24
	Figure 11: Diagrammatic representation of working principle of PXRD.	25
	Figure 12: Diagrammatic representation of working principle of SEM.	26
CHAPTER IV	Figure 1: Plot of ϕ_v^0 versus molality (m) of aqueous BTEAC solutions and as a function of temperature (T/K).	93
	Figure 2: B plotted as a function of temperature (T/K) and different concentrations (m) of aqueous BTEAC solutions.	93
	Figure 3: Plot of limiting molar refractive index (R_M^0) as a function of different molality of aqueous BTEAC solutions and as a function of temperature (T/K).	94
	Figure 4: Plot of molar conductance as a function of the concentration of Amino acids taken in various molality of aqueous BTEAC in solutions at 298.15 K.	94

CHAPTERS	TABLES	PAGE NO.
	Figure 5: Plot of molar conductance as a function of the concentration of Amino acids taken in various molality of aqueous BTEAC in solutions at 303.15 K.	95
	Figure 6: Plot of molar conductance as a function of the concentration of Amino acids taken in various molality of aqueous BTEAC in solutions at 308.15 K.	95
	Figure 7: Plot of molar conductance as a function of the concentration of Amino acids taken in various molality of aqueous BTEAC in solutions at 313.15 K.	96
	Figure 8: Plot of Surface Tension (σ) of L-Alanine and L-Isoleucine as a function of different concentration (molality) of aqueous BTEAC solutions at 298.15 K.	96
	Figure 9: Benesi-Hildebrand double reciprocal plot of (a) BTEAC+L-Alanine (b) BTEAC+L-Isoleucine system.	97
	Figure 10: Double reciprocal plot by using Benesi-Hildebrand Method to obtain Slope and intercept of the straight line at 298.15 K Temperature for (a) BTEAC+L-Alanine and (b) BTEAC+L-Isoleucine system.	97
	Figure 11: ^1H NMR spectra of pure BTEAC (Picture 1), L-Alanine (Picture 2) and L-Isoleucine (Picture 3) in D_2O .	99
	Figure 12: ^1H NMR spectra of BTEAC + L-Alanine (Picture 4) and BTEAC + L-Isoleucine (Picture 5) in D_2O .	100
	Figure 13: Optimized geometries for the (a) BTEAC+L-Alanine (b) BTEAC+L-Isoleucine.	101
	Figure 14: Electrostatic potential maps for (a) L-Alanine+BTEAC (b) L-Isoleucine+BTEAC complexes.	101
	Figure 15: Plots of reduced density gradient (RDG) against electron density multiplied by the sign of the second Hessian eigen value ($\text{sign}(\lambda_2)\rho(r)$) for (a) L-Alanine+BTEAC (b) L-Isoleucine+BTEAC.	102
CHAPTER V	Figure 1: Plot of Limiting apparent molar volume (ϕ_v^0) for two different AAs vs. Molality of MEPN in aqueous solution (or concentration) / mol.kg^{-1} with the variation of temperature (in K).	139
	Figure 2: Viscosity B-Coefficient of two individual AAs vs. Change in molality of aqueous MEPN (or concentration) / mol.kg^{-1} at altered temperatures (in K).	140

CHAPTERS	TABLES	PAGE NO.
	Figure 3: Change of limiting molar refraction (R_m^0) vs. altered molality of MEPN in aqueous solution (or concentration) /mol.kg ⁻¹ with the variation of temperatures (in K).	141
	Figure 4: Double reciprocal plot is shown according to Benesi-Hildebrand for (a) MEPN + L-Val and (b) MEPN + L-Phe system.	141
	Figure 5: Proton NMR spectra of pure MEPN (Pic. 1), L-Phe (Pic. 2), and L-Val (Pic. 3) in D ₂ O.	142-143
	Figure 6: Proton NMR spectra of MEPN + L-Phe (Pic. 4) and MEPN + L-Val (Pic. 5) in D ₂ O.	143-144
	Figure 7: Optimized geometries regarding the (a) L-Val-MEPN (b) L-Phe-MEPN composite systems.	144
	Figure 8: Electrostatic potential maps regarding (a) L-Val-MEPN (b) L-Phe-MEPN composite system.	145
	Figure 9: Simulated absorption spectra (a) L-Val-MEPN (b) L-Phe-MEPN composite system.	145
	Figure 10: Plots of reduced density gradient (RDG) against electron density multiplied with a sign of the second Hessian eigen value ($\text{sign}(\lambda_2)\rho(r)$) regarding (a) L-Val-MEPN (b) L-Phe-MEPN composite systems.	146
	Figure S1: Graph of change in molar conductivity (Λ) vs. concentration of studied AAs in various concentrations of MEPN in aqueous solution at $T=298.15$ K.	146
	Figure S2: Graph of change in molar conductivity (Λ) vs. concentration of studied AAs in various concentrations of MEPN in aqueous solution at $T=303.15$ K.	147
	Figure S3: Graph of change in molar conductivity (Λ) vs. concentration of studied AAs in various concentrations of MEPN in aqueous solution at $T=308.15$ K.	147
	Figure S4: Graph of change in molar conductivity (Λ) vs. concentration of studied AAs in various concentrations of MEPN in aqueous solution at $T=313.15$ K.	148
	Figure S5: Surface tension (σ) plot of L-Val vs. different concentration (molality) of MEPN in aqueous solutions.	148
	Figure S6: Surface tension (σ) plot of L-Phe vs. concentration (molality) of MEPN in aqueous solutions.	149

LIST OF FIGURES

CHAPTERS	TABLES	PAGE NO.
CHAPTER VI	Figure 1: ^1H -NMR spectra of (a) β -CD (b) BB and (c) BBIC in D_2O solvent.	176
	Figure 2: FTIR spectra of (a) β -CD, (b) pure BB, and (c) BBIC inclusion complex.	177
	Figure 3: (a) Alternation of UV-Vis spectra for the generation of Job's plot and (b) Job's plot for BB+ β -CD system at 298.15 K at $\lambda_{\text{max}} = 630$ nm.	177
	Figure 4: Variation in the surface tension of aqueous BB with increasing concentration of β -CD at 298.15 K.	178
	Figure 5: Variation in the conductance of aqueous BB with increasing concentration of β -CD.	178
	Figure 6: Powder XRD spectra of (a) BB, (b) β -CD, and (c) BBIC.	179
	Figure 7: Absorption spectra of 10 μM BB in various concentrations (20 μM to 130 μM) of aqueous β -CD.	179
	Figure 8: Benesi-Hildebrand double reciprocal plot for the effect of β -CD on the absorbance of BB (630 nm) at 298.15 K (X-axis = $1/[\beta\text{-CD}]$ and Y-axis = $1/\Delta A$).	180
	Figure 9: (a) Fluorescence spectra of 10 μM BB in various concentrations of aqueous β -CD and (b) Benesi-Hildebrand double reciprocal plot of $1/F_0 - F$ vs. $1/[\beta\text{-CD}]$ at 298.15 K.	180
	Figure 10: (a) Fluorescence spectra for the generation of Job's plot and (b) Job's plot for BB+ β -CD system at 298.15 K at $\lambda_{\text{max}} = 664$ nm by Fluorescence study.	181
	Figure 11: SEM morphological images of (a) β -CD (b) BB and (c) BBIC.	181
	Figure 12: Several SEM images of BBIC.	181
	Figure 13: (A) UV-visible spectra of BB, exposed to sunlight for 3 hours, (16.2 μM). (B) UV-visible spectra of BBIC, exposed to sunlight for 3 hours (16.2 μM).	182
	Figure 14: (A) Photo degradation % of BB, exposed to sunlight 3 h, (16.2 μM). (B) Photo degradation % of BBIC, exposed to sunlight 3 h (16.2 μM).	182
	Figure 15: UV-Vis spectra of (a) BB and (b) BBIC at different concentrations of CT-DNA.	183
	Figure 16: Percentage of cytotoxicity at different	183

CHAPTERS	TABLES	PAGE NO.
	concentrations of BB and BBIC in the A549 cell line.	
	Figure 17: Percentage of cell viability at different concentrations of BB and BBIC in HEK-293 cell line.	184
	Figure 18: Geometry optimization of the molecules at M06-2X-/6-31+G(d) level of theory. Top and side views of the BB- β -CD.	184
	Figure 19: Geometry of BB- β -CD inclusion complex with calculated major structural parameters were recorded.	185
	Figure 20: HOMO and LUMO charge densities of BB- β -CD inclusion complex.	185
	Figure 21: Electrostatic potential map for BB- β -CD inclusion complex.	186
	Figure 22: Plots of reduced density gradient (RDG) for BB- β -CD inclusion complex.	186
	Figure S1: Absorption spectra of 7.5 μ M BB in 1 μ M to 12 μ M concentration of aqueous β -CD.	187
	Figure S2: Benesi-Hildebrand double reciprocal plot for the effect of lower concentrations β -CD (1 μ M to 12 μ M) on the absorbance of BB (630 nm) at 298.15 K (X axis = $1/[\beta\text{-CD}]$ and Y axis = $1/\Delta A$).	187
	Figure S3: Absorption spectra of 7.5 μ M BB in 150 μ M to 750 μ M concentration of aqueous β -CD.	188
	Figure S4: Benesi-Hildebrand double reciprocal plot for the effect of lower concentrations β -CD (150 μ M to 750 μ M) on the absorbance of BB (630 nm) at 298.15 K (X axis = $1/[\beta\text{-CD}]$ and Y axis = $1/\Delta A$).	188
	Figure S5: Fluorescence emission decay of BB and BBIC.	189
CHAPTER VII	Figure 1: (a) Changes of UV-Vis Spectra for the generation of Job's plot and (b) Job's plot for VC- γ -CD complex at 298.15 K.	214
	Figure 2: ^1H -NMR spectra of (a) γ -CD (b) VC and (c) ICVC in D_2O solvent.	215
	Figure 3: FTIR spectra of (a) VC, (b) γ -CD, and (c) ICVC.	216
	Figure 4: Variation in the aqueous VC conductance with increasing concentration of γ -CD.	217
	Figure 5: Variation in the surface tension of aqueous VC	218

LIST OF FIGURES

CHAPTERS	TABLES	PAGE NO.
	with increasing concentration of γ -CD at 298.15 K.	
	Figure 6: (a) Absorption spectra of 100 μ M VC in different concentrations (10 μ M to 110 μ M) of aqueous γ -CD (b) Benesi-Hildebrand double reciprocal plot for the effect of γ -CD on the absorbance of VC ($\lambda_{\text{max}} = 252 \text{ nm}$) at 298.15 K (X-axis = $1/[\gamma\text{-CD}]$ and Y-axis = $1/\Delta A$).	218
	Figure 7: SEM images of (a) Valacyclovir (VC) (b) γ -Cyclodextrin (γ -CD) (c) Inclusion complex (ICVC).	218
	Figure 8: UV-visible spectra of (a) ICVC and (b) VC exposed to sunlight for 3 hours.	219
	Figure 9: Photo degradation % of (a) ICVC and (b) VC exposed to sunlight for 3 hours.	219
	Figure 10: FTIR spectra of pure drug VC, ICVC, Carbopol 940, gel without drug, VC loaded gel, ICVC loaded gel.	220
	Figure 11: Zeta potential value of (A) pure VC-loaded gel and (B) ICVC-loaded gel.	220
	Figure 12: Percentage cumulative VC release from pure VC-loaded gel and ICVC-loaded gel.	221
	Figure 13: Ex-vivo permeation of VC from VC-loaded gel and ICVC-loaded gel.	221
	Figure 14: Optimized structure of the supramolecular complex ICVC (a) side view (b) top view.	222

LIST OF SCHEMES

CHAPTERS	SCHEMES	PAGE NO.
CHAPTER IV	Scheme 1: The molecular structure of L-Alanine, L-Isoleucine and Benzyltriethylammonium chloride.	102
	Scheme 2: Plausible molecular interactions between Ionic Liquid and Amino acids, (a) & (d) Ion-Ion interaction, (b) & (e) Hydrophobic-Hydrophobic interaction, (c) & (f) Ion-Hydrophobic interaction.	103
CHAPTER V	Scheme 1: Molecular structures of L-Valine (a), L-Phenylalanine (b) and Mephnesin (c).	149
	Scheme 2: Plausible sketches of various patterns shown for molecular interactions associate with MEPN drug in presence of two AAs L-Val and L-Phenylalanine: (a) and (d) Hydrophobic-Hydrophobic interactions; (b) and (e) Ion-Dipole interaction; (c) and (f) Ion-Hydrophobic interactions as well as π - π interaction in case only (f).	150
CHAPTER VI	Scheme 1: 2D Molecular structure of (a) Brilliant Blue FCF (BB) and (b) Beta-cyclodextrin (β -CD).	189
	Scheme 2: Schematic diagram for the formation of BBIC inclusion complex of Brilliant Blue FCF with Beta-cyclodextrin.	189
CHAPTER VII	Scheme 1: 2D Molecular structure of (a) Valacyclovir Hydrochloride (VC) and (b) Gamma-Cyclodextrin (γ -CD) and (c) Schematic diagram for the formation of inclusion complex (ICVC).	223

ABBREVIATIONS

CD	Cyclodextrin
β -CD	Beta Cyclodextrin
γ -CD	Gamma Cyclodextrin
IC	Inclusion complex
BTEAC	Benzyltriethylammonium chloride
MEPN	Mephenesin
L-Val	L-Valine
L-Phe	L-Phenylalanine
BB	Brilliant Blue FCF
BBIC	Inclusion complex of Brilliant Blue FCF with β -CD
HEK-293	Human embryonic kidney cell line
A-549	Human adeno carcinomic alveolar basal epithelial cell
VC	Valacyclovir
ICVC	Inclusion complex of Valacyclovir
FMO	Frontier Molecular Orbital
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
PCM	Polarizable Continuum Model
NCI	Non-Covalent Interaction
IL	Ionic liquid
AA	Amino acid
CT-DNA	Calf Thymus DNA
ESP	Electrostatic potential
RDG	Reduced density gradient
DFT	Density functional Theory
μm	Micrometre
$\text{\AA}$	Angstrom
C	Carbon

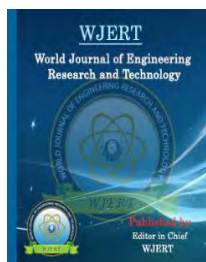
ABBREVIATIONS

H	Hydrogen
O	Oxygen
cm	Centimetre
Eq.	Equation
eV	Electron Volt
g	Gram
hrs	Hours
Hz	Hertz
FTIR	Fourier Transform Infrared spectroscopy
K	Kelvin
M	Molar
m	Molal
mg	Milligram
min	Minute
mL	Millilitre
μ M	Micromolar
$^{\circ}$ C	Degree Celsius
pH	Potential of Hydrogen
rpm	Revolutions Per Minute
SEM	Scanning Electron Microscopy
UV-vis	Ultraviolet-visible
NMR	Nuclear Magnetic Resonance
PXRD	Powder X-Ray Diffraction

APPENDIX-A

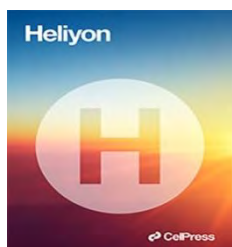
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1. **B. Saha**, S. Barman, S. Majumder, N. Roy, B. Ghosh, R. Chakrabarty, S. Choudhury, N. N. Ghosh, K. Baul and M. N. Roy, Physicochemical studies of biologically potent molecules in aqueous ionic liquid solutions with the manifestation of solvation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



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

2. **B. Saha**, S. Barman, S. Majumder, B. Ghosh, K. Mallick, S. Choudhury, M. N. Roy, Investigation of intermolecular interactions of L-Valine and L-Phenylalanine with muscle relaxant drug mephenesin molecule prevalent in aqueous solution by various physico-chemical methods at T=298.15K–313.15K.



Heliyon 10, (2024) e23562
(Included in the Thesis)

3. **B. Saha**, S. Barman, M. Mondal, S. Choudhury, S. Saha, P. Bomzan, S. Ali, K. Mallick, A. Dutta, A. Kumar, S. Bhattacharjee, M. N. Roy, Exploring Brilliant Blue FCF Assembly with Beta Cyclodextrin, Characterizations and Applications in Biological Systems Using Physicochemical and Computational Methods.



ChemistrySelect 9, (2024) e202302895
(Included in the Thesis)

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4. 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

5. K. Mallick, M. Mondal, D. Roy, P. Roy, S. Ali, D. Roy, **B. Saha**, S. Choudhury, S. Debnath, N. Roy, S. Saha, M. N. Roy, Exploring Various Molecular Interactions of Two Essential Amino Acids Prevalent in Aqueous Solutions of an Ionic Liquid by Density, Viscosity, Refractive Index, Conductance, Surface Tension, Nuclear Magnetic Resonance, Ultraviolet, and Computational Studies.



Journal of Chemical & Engineering Data, 68, (2023) 3045–3061

6. D. Roy, S. Majumder, K. Mallick, N. Roy, **B. Saha**, S. Saha, B. Sinha, Exploration of Solvation Consequences of Ionic Liquids Prevalent in the Aqueous Media of Food Additive Azo Dye Tartrazine by Physicochemical and Computational Studies.



Journal of Chemical & Engineering Data, 69, 1, (2024) 38–58

7. S. Barman, **B. Saha**, S. Majumder, K. Roy, T. Ray, L. Sarkar, A. Sinha, M. N. Roy, Solvation Consequences of Some Noteworthy Molecules in Diverse Liquid Environments Explored by Physicochemical Methodologies.



Journal of Chemical, Biological and Physical Sciences, 12, 4, (2022) 337-363

APPENDIX-B

LIST OF SEMINARS/CONFERENCES ATTENDED

1. 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).*
2. 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).*
3. International Conference on “Advances in Plants, Microbes and Agricultural Sciences” Sponsored by: DBT & DST-SERB (Govt. of India) Organised by: Department of Botany, University of North Bengal, 2nd -4th March, 2023. *(Presented a paper).*
4. International Seminar on “Frontiers in Chemistry 2023 & Prof. C. N. R. Rao Endowment Lecture” Organised by: Department of Chemistry, University of North Bengal & CRSI North Bengal Local Chapter, 13-15th March, 2023. *(Presented a poster).*