

*Dedicated*  
*to*  
*My Parents*

## **DECLARATION**

I declare that the thesis entitled "**Design and Development of Synthetic Methodologies for Medicinally Privileged Heterocyclic Scaffolds**" has been prepared by me under the guidance of Dr. Md. Firoj Hossain, Assistant Professor, Department 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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# PREFACE

Heterocyclic compounds are the prime constituent for the designing of medicinally and pharmaceutically active compounds. Besides the therapeutic importance, heterocyclic compounds are also used for the synthesis of pesticides, fungicides, rodenticides, insecticides, and agrochemicals. With the ever-increasing demand to design new medicinally important heterocycles, researchers around the globe using many improved synthetic protocols to meet the need.

The present effort defines newer synthetic methodologies to construct a wide range of medicinally privileged heterocyclic moieties. This thesis commences with **Chapter I**, which provides a concise review of various synthetic protocols for the synthesis of medicinally active heterocyclic compounds. **Chapter II** describes Graphene oxide (GO) catalyzed one-pot multicomponent synthesis of hydrazinyl thiazoles in ethanol medium at room temperature by the reaction of aldehydes/ketones with thiosemicarbazide and phenacyl bromides. **Chapter III** demonstrates the utilization of Choline chloride: glycerol (1:2) based Deep Eutectic Solvent (DES) as a solvent as well as a catalyst for one pot two component synthesis of quinoxaline derivatives by the reaction between *o*-phenylenediamines and phenacyl bromides. **Chapter IV** illustrates one-pot three-component preparation of naphthopyranopyrimidines in a DES medium by mixing aldehydes, with  $\beta$ -naphthol and 6-amino-1,3-dimethyl uracil. **Chapter V** describes the synthesis of pyrimidobenzothiazole via a one-pot three-component reaction of aldehydes, 2-amino benzothiazole, and  $\beta$ -keto ester in a DES medium.

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## **LIST OF APPENDICES**

### **APPENDIX A: List of Research Publications**

### **APPENDIX B: Poster Presentations**

## APPENDIX A

### **List of Publications (Related to Thesis Work)**

1. “Metal-Free One-Pot Synthesis of 2-(2-Hydrazinyl) Thiazole Derivatives Using Graphene Oxide in a Green Solvent and Molecular Docking Studies”, **Arindam Das**, S. Dey, S. Chakraborty, A. Barman, Ram Naresh Yadav, Rabiul Gazi, Madhurima Jana, and Md. Firoj Hossain\*, *ChemistrySelect* 2021, **6**, 9552–9558.
2. “An Expeditious One-Pot Two-Component Synthesis of Quinoxaline Derivatives in Natural Deep Eutectic Solvents (NADESs)”, **Arindam Das**, Sovan Dey, Ram Naresh Yadav, Palash Jyoti Boruah, Prerana Bakli, Sourav Sarkar, Partha Mahata, Amit Kumar Paul, and Md. Firoj Hossain\*, *ChemistrySelect*, 2023, **8**, e202204651
3. “Unleashing Naphthopyranopyrimidine's Anticancer Potential: A Deep Eutectic Solvent (DES) Study”, **Arindam Das**, Sovan Dey, Ram Naresh Yadav, Prajna Dutta, Shubham Dhiman, Palash Jyoti Boruah, Koushik Sarkar, Abhishek Sahu, Anupam Jana, Amit Kumar Paul, and Md. Firoj Hossain\*, *New J. Chem.*, 2024, **48**, 7566-7578.
4. “Deep Eutectic Solvent catalyzed one-pot multicomponent synthesis of 4H-pyrimido [2,1-*b*] benzothiazole derivatives” (Manuscript under preparation)

### **List of Publications (Not Related to Thesis Work)**

1. Synthetic Strategies for Hydrazinyl Thiazole Derivatives, Sovan Dey, Arindam Das, Md. Firoj Hossain\*, *ChemistrySelect* 2020, **5**, 15153–15166.
2. Recognition of monocarboxylic acids by imidazole based fluorescent receptors, Md. Firoj Hossain\*, Arindam Das, Sovan Dey, Sumit Chakraborty, Anup Barman, Ashim Sen and Rinku Chakrabarty\*, *J. Indian Chem. Soc.* 2020, **97(11a)**, 2291-2299.
3. Galiellalactone: a review on synthetic strategies and tactics, Sovan Dey, Arindam Das, and Md. Firoj Hossain\*, *Chem. Pap.*, 2022, **77**, 2329–2342
4. Visible-light-induced ternary electron donor–acceptor complex enabled synthesis of 2-(2-hydrazinyl) thiazole derivatives and the assessment of their antioxidant and antidiabetic therapeutic potential, Sovan Dey, Arindam Das, Ram Naresh Yadav, Palash Jyoti Boruah, Prerana Bakli, Tania Baishya, Koushik Sarkar, Anup Barman, Ranabir Sahu, Biplab Maji, Amit Kumar Paul, and Md. Firoj Hossain\*. *Org. Biomol. Chem.*, 2023, **21**, 1771-1779

5. Synthesis of Cu (II) and Zn (II) Complexes of a Quinoline Based Flexible Amide Receptor as Fluorescent Probe for Dihydrogen Phosphate and Hydrogen Sulphate and Their Antibacterial Activity, Sovan Dey, Sandip Ghosh, Arindam Das, Ram Naresh Yadav, Rinku Chakrabarty\*, Smriti Pradhan, Dipanwita Saha, Ashok Kumar Srivastava, and Md. Firoj Hossain\*. *Journal of Fluorescence*, 2023

## APPENDIX B

### **Poster Presentation**

1. Graphene Oxide (GO) Catalyzed One-Pot Multicomponent Synthesis of 2-(2-Hydrazinyl) thiazole Derivatives and Molecular Docking Studies, **Arindam Das**, Sovan Dey, and Md. Firoj Hossain\*, International Symposium on “Emerging Trends in Chemical Sciences (ETCS-2023)”, Organised by Department of Chemistry, North-Eastern Hill University (NEHU), Shillong, India.
2. One-Pot Synthesis of Quinoxaline Derivatives Using Choline Chloride and Glycerol Based Deep Eutectic Solvent (DES), **Arindam Das** and Md. Firoj Hossain\*, International Seminar on “Frontiers in Chemistry 2023”, Organized by Department of Chemistry, University of North Bengal, Darjeeling, India.

## ABBREVIATION

---

|       |                                         |
|-------|-----------------------------------------|
| ChCl  | Choline chloride                        |
| CPB   | Cetylpyridinium bromide                 |
| CQD   | Carbon quantum dot                      |
| CTAB  | Cetyltrimethyl ammonium bromide         |
| °C    | Degree celsius                          |
| d     | Doublet                                 |
| DABCO | 1,4-diaza bicyclo [2.2.2] octane        |
| DBU   | 1,8-diazabicyclo [5.4.0] undec-7-ene    |
| DCE   | 1,2-dichloro ethane                     |
| DCM   | Dichloromethane                         |
| DES   | Deep eutectic solvent                   |
| DFT   | Density functional theory               |
| DIPEA | N, N-diisopropyl ethylamine             |
| DLS   | Dynamic light scattering                |
| DMF   | N, N-Dimethyl formamide                 |
| DMSO  | Dimethyl sulfoxide                      |
| DSC   | Differential scanning calorimeter       |
| EAA   | Ethyl acetoacetate                      |
| ERG   | Electron releasing group                |
| ESI   | Electrospray ionization                 |
| EWG   | Electron withdrawing group              |
| FT-IR | Fourier transform infrared spectroscopy |
| GO    | Graphene oxide                          |
| h     | hour                                    |
| HBA   | Hydrogen bond acceptor                  |
| HBD   | Hydrogen bond donor                     |
| HOMO  | Highest occupied molecular orbital      |
| HRMS  | High resolution mass spectrometry       |
| Hz    | Hertz                                   |
| IL    | Ionic liquid                            |

|       |                                     |
|-------|-------------------------------------|
| LED   | Light emitting diode                |
| LGA   | Lamarckian genetic algorithm        |
| LUMO  | Lowest unoccupied molecular orbital |
| m     | Multiplet                           |
| MAA   | Methyl acetoacetate                 |
| MCR   | Multicomponent reaction             |
| mg    | Milligram                           |
| MHz   | Mega hertz                          |
| min   | minute                              |
| mL    | millilitre                          |
| mmol  | millimole                           |
| NADES | Natural deep eutectic solvent       |
| NBS   | N-bromo-succinamide                 |
| NMR   | Nuclear magnetic resonance          |
| NP    | Nanoparticle                        |
| OLED  | Organic light-emitting diodes       |
| PEG   | Polyethylene glycol                 |
| q     | Quartet                             |
| RMSD  | Root mean square deviation          |
| rGO   | Reduced graphene oxide              |
| rt    | Room temperature                    |
| s     | Singlet                             |
| SEM   | Scanning electron microscopy        |
| t     | Triplet                             |
| TBAHS | Tetrabutylammonium hydrogen sulfate |
| TBHP  | Tert-butylhydroperoxide             |
| TEM   | Transmission electron microscopy    |
| TGA   | Thermogravimetric analysis          |
| TLC   | Thin layer chromatography           |
| TMS   | Tetramethylsilane                   |
| VSM   | Vibrating sample magnetometer       |
| XRD   | X-ray diffraction                   |