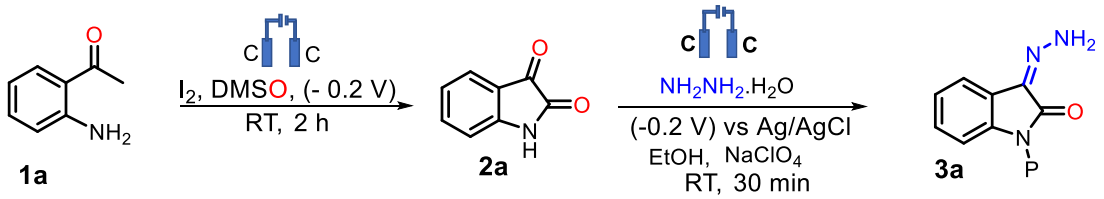
Summary and Conclusions

The thesis entitled **"A Novel Approach for the Synthesis of *N*-based Heterocyclic Compounds and their Electrochemical Studies"** described the effective green synthesis of biologically active *N*-containing heterocyclic compounds. The content of the thesis has been divided in to six chapter.

Chapter 1 Provide a detailed explanation of electro-organic synthesis and its significance in organic synthesis, *N*-containing heterocycles and their importance, and different methods synthesizing *N*-containing compounds. The following four chapters describe the studies and conclusions (Chapter 2 through 5). Each chapter, which is utterly complete in itself, consist of an introduction, result and discussion, controlled experiment, mechanism, experimental section, and references.

Chapter 2 describe a simple, green, eco-friendly, highly efficient, inexpensive process for the synthesized isatins and their respective hydrazones in good to excellent yields using an electro-organic synthetic approach through C–N cross-coupling and C(sp^2)–H/C(sp^3)–H functionalization. In our initial studies, we took 2-aminoacetophenone **1a** as amodel substrate to probe various reaction parameters in an undivided cell, we have chosen graphite electrodes for our study as graphite electrodes have advantages over other electrodes by offering excellent conductivity, homogeneity, stability, large surface area, versatility, chemical inertness and cost-effectiveness, all of which are crucial for the electrochemical process.

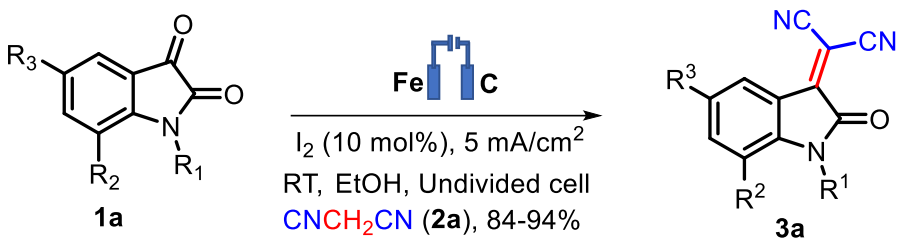


Scheme 6.1 Synthesis of isatin hydrazones.

- ✓ **Short reaction time**
- ✓ **Low yield of the product**
- ✓ **Easy Isolation**
- ✓ **Green Solvent**
- ✓ **Room temperature reaction, environment friendly solvent**

We first evaluated the requirement of a promoter and the choice of solvent using *n*-BuNBr as the electrolyte at a constant voltage of −0.2 V under ambient atmosphere for **2h** in an undivided cell equipped with graphite carbon (2 cm^2) both as an anode and a cathode at room temperature (25 ℃).

Chapter 3 describes a mild, efficient, Isatylidene malononitrile, also known as the 2-(2 oxoindolin-3-ylidene) malononitrile, is an intriguing michael acceptor that is used to build possible bioactive compounds. The development of novel construction techniques for 2-(2-oxoindolin-3-ylidene) malononitrile has garnered significant attention due to its distinct structural characteristics and intriguing biological attributes. The synthesis of isatylidene malononitrile-based structures is of general interest due to its biological uses and structural features. we herein report a three-component reaction using isatin **1a** (1.0 mmol), malononitrile **2a** (1.0 mmol), and iodine (10 mol%) in ethanol (20 mL) to furnish the desired isatylidene malononitrile **3a** in 94% isolated yield

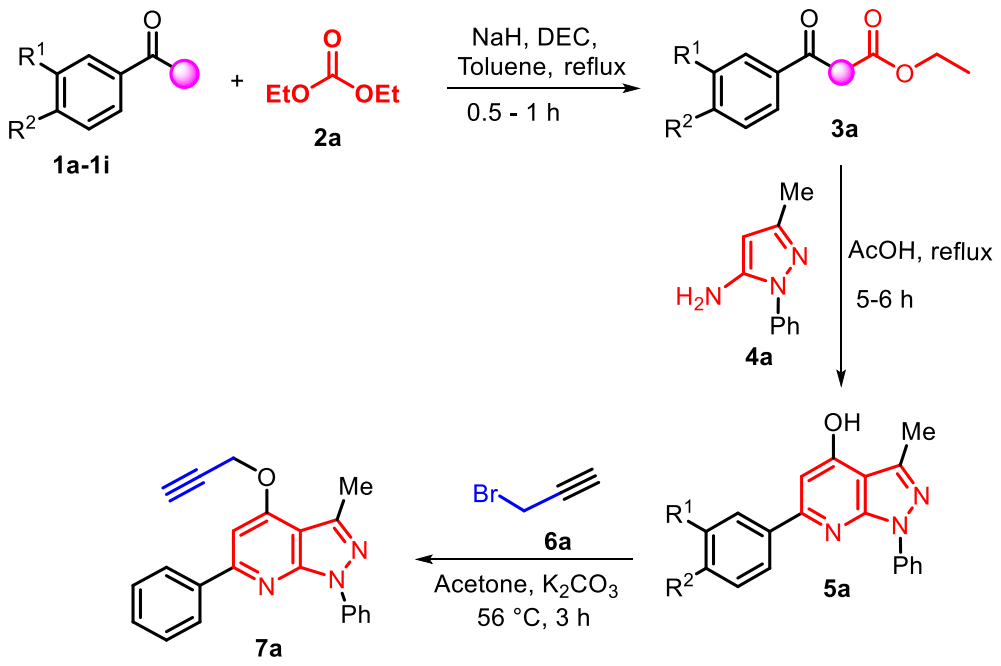


Scheme 6.2 Synthesis of 2-(2-oxoindolin-3-ylidene) malononitrile.

- ✓ **Short reaction time**
- ✓ **New C=C bond formation**
- ✓ **Easy Isolation**
- ✓ **Green Solvent**
- ✓ **Room temperature reaction, environment friendly solvent**

The electrochemical synthesis was carried out in an undivided cell equipped with carbon cloth (2 cm^2) as an anode and iron (2 cm^2) as a cathode at room temperature under a constant current density of 5 mA cm^{-2}. OCP was observed for different isatin derivatives, electro-organic synthesis reaction mixture in a potential region of +1 V to -1 V.

Chapter 4 describes a cost-effective and competent approach has been established for the synthesis of *N*-heterocyclic compounds have a crucial function in facilitating biological function in cancer and deserve more attention some *N*-heterocyclic compounds, such pyrazolo[3,4-b] pyridine, have been discovered to be more effective than others at boosting biological activity heterocyclic compounds such as derivatives of pyrazolo-pyridine and pyrazolo-pyrimidine are privileged bioactive compounds. The number of these molecules have shown useful as antienteroviral drugs, antimalarial drugs, anticancer drugs and kinase inhibitors Initially, we commenced our strategy for the synthesis of various pyrazolo[3,4-b] pyridines starting from β-keto esters followed by propargylation of pyrazolo pyridine-7-ol was planned, and the retrosynthetic route is presented in **Scheme C** to achieve the synthesis of designed, targeted compounds. Further, the electrochemical technique of cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) is widely used to study the reduction, oxidation, and charge transfer process of molecular species.

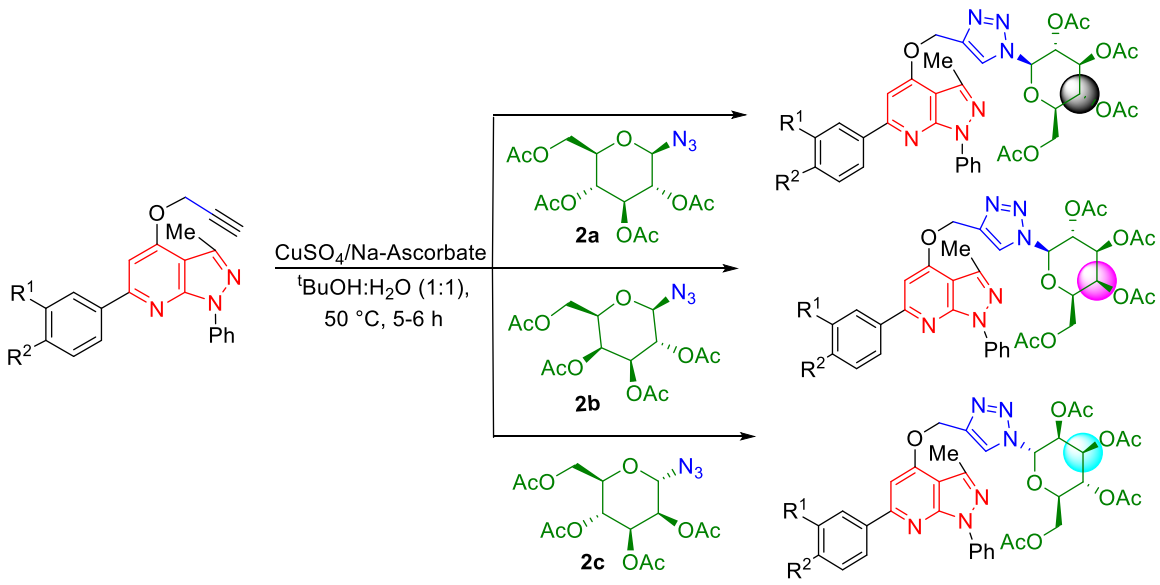


Scheme 6.3 Synthesis of propargylation of pyrazolo-pyridine-7-ol.

- ✓ **Short reaction time**
- ✓ **Functional group tolerance**
- ✓ **Easy Isolation**
- ✓ **Excellent yield**

Chapter 5 describes a phrase "click chemistry" was first used in 2001 by chemist K. Barry sharpless to characterize a group of facile, potent, highly selective and modular reactions. Reactions that are dependable and selective are at the core of click chemistry and are therefore ideal for a variety of chemical and biological applications. Azido glycosides were utilized as building blocks in a wide variety of biochemical processes, including the production of amino sugars, glucosamines, neoglycoconjugates (including *N*-glycopeptides, *N*-glycoproteins, heterocyclic compounds, and more)**.** Staudinger reduction, Curtius and Schmidt rearrangements, and 1,3-dipolar cycloaddition are few examples of the chemical processes in which azido glycosides play a significant role.

The first 'click chemistry' reaction of propargyl pyrazolo-pyridine-7-ol **3a** with 1-azido-2,3,4,6-tetra-*O*-acetyl β-D-glucose **2a** was performed under thermal conditions (50 °C) in ^{t}BuOH: H_2O (1: 1) for 6 hours using $CuSO_4.5H_2O$ and sodium ascorbate, and it furnished the desired 1,2,3-triazole linked *N*-glycosides of pyrazolo-pyridine in 95% isolated yields with some recovered starting material **Scheme 6.4.**



Scheme 6.4 Synthesis of propargylation of pyrazolo-pyridine-7-ol.

- ✓ **Short reaction time**
- ✓ **High yield of the product**
- ✓ **Easy Isolation**
- ✓ **Biologically active molecule**

Thus, 1,2,3-triazole linked galactohybrids pyrazolo pyridines was obtained in very good isolated yield (92%) in a highly regioselective manner in just 6 hours when a similar reaction was carried out in a conventional method at 50 °C in the presence of $CuSO_4.5H_2O$ and sodium ascorbate in ^{t}BuOH: H_2O (1: 1). We hoped that by employing traditional aided click-chemistry, we might speed up the reaction, obtain the desired

products in less time, and improve the yields. The product was confirmed by the electrochemical (CV and EIS) technique.

Scope for Future Work

1. Electro-organic synthesis refers to the use of electrical energy to drive chemical reactions involving organic compounds. This approach has gained attention in recent years due to its potential for more sustainable and environmentally friendly synthesis processes.
2. Further, explore the electro-organic synthesis future developments may involve integrating electro-organic synthesis with other synthetic methodologies. Combining electrochemical methods with traditional organic synthesis or other emerging technologies could lead to synergistic effects, enabling the creation of complex molecules in a more streamlined and efficient manner.
3. Continued collaboration between researchers, industry stakeholders, and policymakers will be essential to drive innovation, overcome challenges, and realize the full potential of electro-organic synthesis in the future.