



Benzimidazole Derivative Synthesis via Visible-Light Photo-Redox: An Eco-Friendly Path to Bioactive Heterocyclic



Swatantra Bajpai, Nidhi Srivastava

Abstract: Using visible-light-induced photo-redox catalysis, a sustainable and environmentally friendly method for the synthesis of benzimidazole-based heterocyclic compounds has been established. Under green LED irradiation ($\lambda = 535 \text{ nm}$, 18 W) in tetrahydrofuran (THF) at room temperature, the procedure uses Eosin Y as an effective, metal-free photosensitizer. Eosin Y (1 mol%) and THF performed best, according to optimization experiments, yielding the target product 2-(furan-2-yl)-1H-benzimidazole in an isolated yield of 82% after 70 minutes. The process involves photoexcitation of Eosin Y, generation of radicals, and subsequent formation of a benzimidazole derivative via a single-electron transfer (SET) pathway. IR, ^1H NMR, ^{13}C NMR, and ESI-MS investigations verified the product structure. This green LED-mediated technology has several advantages over traditional thermal approaches, including great atom economy, energy efficiency, metal-free operation, and quicker reaction times.

Keywords: Eosin-Y photo Redox Process, Benzimidazole Photo Redox Reaction, Heterocycles, Bioactive Substances, Green Chemistry, and Visible Light.

Nomenclature:

SET: Single-Electron Transfer

TLC: Thin-Layer Chromatography

THF: Tetrahydrofuran

I. INTRODUCTION

In many scientific and industrial fields, including organic synthesis, agrochemical chemistry, and pharmaceutical chemistry, heterocyclic compounds constitute one of the most important and broad categories of organic molecules. (Javahershenas et al.2024) [1]. These compounds' ring structures include heteroatoms such as oxygen, nitrogen, or sulfur, which confer unique chemical and biological properties. Heterocyclic chemistry is thus in constant demand as a main field of organic synthesis due to the development of new medicines and useful materials. (Qadir et al.2022) (Obaid et al.2022) [2-3]. Given their diverse biological and pharmacological properties, benzimidazoles have held a prominent position among heterocyclic compounds.

Benzimidazole derivatives are really good at working with living things.

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This makes Benzimidazole derivatives useful for creating new medicines. Benzimidazole derivatives can do many things. They can help fight cancer, bacteria, malaria, viruses, fungi, parasites and inflammation. Benzimidazole derivatives are very good at this. They can even help with other things. This is why people like to use Benzimidazole derivatives when they make therapeutic agents. (Brishty et al.2021) [4-6].

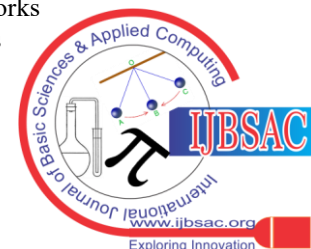
This versatility makes them important in drug discovery and development; therefore, extensive research is underway to synthesise benzimidazole derivatives with improved pharmacological properties and biological effects (Pandey et al., 2022) [7]. However, the term "typical creation" refers to benzimidazole compounds.

Benzimidazole compounds have traditionally been produced under refluxing circumstances using thermal cyclisation and condensation techniques. (Aroua et al. 2025) [8]. Even though these procedures frequently produce the intended results, they usually require elevated temperatures, long reaction periods, and occasionally metal catalysts, which raise energy and environmental concerns. (Banerjee et al.2025) (Green synthesis methods et al.2026) [9-10].

For example. Reaction conditions: 1.0 mmol of aldehyde (furfural), 1.0 mmol of o-phenylenediamine, 0.1 mol% of copper-substituted zinc aluminate catalyst, 5 mL of water, room temperature (Kadam-U. D et al, 2025) [11].

Using visible light as a plentiful and renewable energy source, visible-light photo-redox catalysis has become a sustainable and environmentally friendly method in organic synthesis in recent years, enabling the production of reactive intermediates under mild conditions. (Sharma et al. 2023) [12]. As metal-free photosensitizers, organic dyes such as Rhodamine B, Rose Bengal, and Eosin- Y have been used extensively to promote single-electron transfer (SET) processes that facilitate the formation of C–C and C–heteroatom bonds. (Ferlin et al. 2023) [13-15]. Using visible light improves reaction selectivity and operational simplicity while reducing environmental impacts. (Rai et al.2024) [16].

Despite the abundance of research on visible-light-induced C–C bonding and cyclisation processes, the photoinduced synthesis of benzimidazole analogues remains little known. In this context, we have developed a photoinduced, metal-free, and energy-efficient approach to the synthesis of benzimidazole-based heterocyclic compounds via visible-light irradiation of furfural. The single-electron transfer mechanism is what drives the reaction. This method is good for the environment because it works at room temperature. It also makes the reaction happen faster, gives



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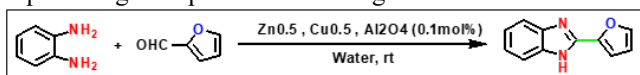
the product, and uses the atoms more efficiently.

This work provides a method for the synthesis of environmentally friendly, sustainable benzimidazole derivatives. The single-electron transfer mechanism and light photo redox catalysis are key to this process. Light photo-redox catalysis shows promise for creating new heterocycles that can be used as medicine. The single-electron transfer mechanism and light photo redox catalysis are important for the synthesis of bioactive benzimidazole derivatives.

A. Previous Work

The combination of heterocyclic compounds based on benzimidazoles was previously observed using a traditional heating approach involving the reaction of furfural with benzene-1,2-diamine. At room temperature, the process proceeded in the presence of a Zinc aluminate catalyst with copper substitution (0.1 mol%) and water (5 mL) to yield the corresponding derivative of Furan-associated benzimidazole (Scheme 1.1).

This process produced the necessary results, but it was energy-intensive and less environmentally friendly because it required high temperatures and long reaction times.



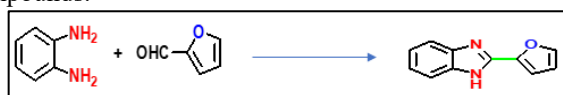
Scheme 1.1: Furfural is Used in the Heated Synthesis of a Benzimidazole Derivative

B. Present Work

Furfural was used in a photoinduced synthesis of benzimidazole-based heterocyclic compounds under visible-light irradiation, building on earlier research. This approach was developed as a sustainable, environmentally friendly alternative to traditional thermal techniques.

The reaction was conducted under mild conditions at room temperature with an organic solvent (THF) and a metal-free photosensitizer (eosin Y). Through a single-electron transfer (SET) mechanism, the transition was facilitated by visible light, which promoted the formation of an imine intermediate and the coupling of benzimidazole compounds (Scheme 1.2).

This visible-light-induced method is a sustainable and effective way to synthesise benzimidazole derivatives, offering several benefits, including metal-free operation, shorter reaction times, lower energy consumption, and high product yields. Following the principles of green chemistry, the process demonstrates that visible-light photo-redox catalysis can be a useful, environmentally responsible alternative for the development of bioactive heterocyclic compounds.



[Scheme 1.2: Photoinduced Synthesis of Benzimidazole Derivative Using Furfural Under Visible Light Conditions]

II. EXPERIMENTAL SECTION

A. Materials

There was no need for additional purification, as all analytical-quality reagents and solvents were utilised precisely as supplied by commercial vendors. Furfural (C₅H₉O₂), benzimidazole (C₇H₆N₂), eosin Y, and

tetrahydrofuran (THF) were provided by Merck and CDH Chemicals. Before using the glassware, we made sure it was completely dry by placing it in the oven. We also used water with all the bad stuff removed when needed.

B. Basic Method for Benzimidazole Derivatives Photoinduced Synthesis

Benzimidazole (0.5 g, 0.007 mol) and furfural (1.5 g, 0.01 mol) were combined in a 100 mL round-bottom flask and dissolved in 10 mL of tetrahydrofuran (THF). Eosin Y (0.006 g, 2 mol%) was then added as a photosensitizer. The reaction mixture was stirred under visible green LED light ($\lambda = 535$ nm, 18 W) at room temperature (approximately 25 °C) for 70 minutes. During the reaction, the colour changed from white to yellow, indicating product formation. The reaction proceeded with benzimidazole and furfural in the presence of Eosin Y under light irradiation. After 70 minutes, the product was obtained.

C. Measuring the Improvement of Reactions

Utilising ethyl acetate: methanol (9:1, v/v) as the mobile phase, thin-layer chromatography (TLC) on silica gel standard plates was used to monitor the reaction's progress. Under UV light (254 nm), spots were visible. The absence of the starting material confirmed that the reaction had stopped.

D. Purification

The reaction mixture was concentrated at reduced pressure using a rotating evaporator after completion. Ethyl acetate was used as the eluent in silica gel column chromatography (mesh size 100–200) to purify the crude product. A light-yellow crystalline solid was produced by combining fractions containing the pure chemical (TLC confirmed) and condensing them until they were totally dry.

E. Characterisation Data

2-(furan-2-yl)-1H-benzimidazole: White to off-white crystalline yellow solid; Yield: 82%; M.P.: 280-90°C, R_f = 0.55 - 0.65. Benzene: Ethanol (8:2)

¹H NMR (400 MHz, DMSO-d₆):

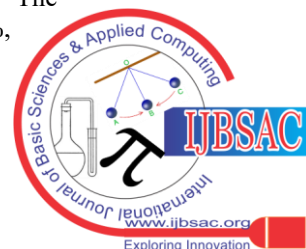
δ 12.12 (bs, 1H, -NH), 7.50–7.60 ppm (m, 2H), 7.0–7.2 ppm (m, 2H), 7.85–7.90 ppm (dd, J = 1.7 Hz, J = 0.8 Hz, 1H), 7.20–7.21 ppm (d, J = 3.2 Hz or 4.0 Hz, 1H), and 6.5–6.7 ppm (dd, J = 3.1 Hz, J = 1.7 Hz, 1H).

¹³C NMR (400 MHz, DMSO-d₆): δ 152.0, 142.6, 143.6, 140.5, 131.8, 121.6, 117.5, 111.8, and 110.5 ppm.

ESI-MS(m/z): 184 M⁺ ([M+H]⁺ base peak), 183, 155, 129, 103, 77

III. FINDINGS AND CONVERSATION

A series of systematic control experiments was conducted to optimise response parameters in the visible-light-induced synthesis of standard benzimidazole heterocyclic compounds. In the model reaction, furfural (1.5 g, 0.01 mol) and benzene-1,2-diamine (0.5 g, 0.007 mol) were combined in tetrahydrofuran (THF, 10 mL) with eosin Y (1 mol%) as the photocatalyst under ambient temperature and green LED irradiation ($\lambda = 554$ nm, 18 W). The reaction progress was monitored at regular intervals. The highest conversion and yield, 82%, were achieved after 70 minutes of irradiation, indicating that this





duration is optimal for the reaction (Table I, Entry 1).

A. Optimization of Reaction Conditions

A range of organic dyes, including Rose Bengal, Rhodamine B, and Eosin Y, was tested under identical conditions to identify the most efficient photocatalyst. With the highest production (82%) of the required benzimidazole derivative, Eosin Y outperformed the others when exposed to green LED light (Table I, Entry 1). Eosin Y's exceptional spectrum overlaps with green light, increasing its excitation to the triplet state and promoting an efficient single-electron transfer (SET) process that underlies its outstanding efficiency. The impact of several solvents on reaction efficiency was next investigated (Table I, Entries 1–9). THF was found to be the best solvent, yielding the product with outstanding yield and purity. The great solubility of both reagents and the effective stabilization of the stimulated-state photocatalyst in THF are the reasons for this. As the photocatalyst loading increased, 1 mol% Eosin Y was sufficient to achieve full conversion. Therefore, the optimized conditions for the photoinduced synthesis were determined as follows:

THF (10 mL), green LED (18 W), Eosin Y (1 mol%), and a 70-minute reaction time at room temperature (25 degrees Celsius). The furan-linked benzimidazole compound was produced in 82% yield under these conditions, a significant improvement over the previously used red-light process.

B. Proposed Mechanism

A possible photo-redox catalytic system for green-light-induced reaction is shown in Scheme 3.1. Upon getting excited to the single-molecule state of excitement ($^1EY^*$) by stimulation to green LED light, Eosin Y conducts intersystem crossover to attain a triplet excited state ($^3EY^*$). This photoexcited dye acts as a single-electron transfer (SET) catalyst, reducing furfural to create a radical and changing into its radical anion form ($EY^{\bullet-}$). At that, the radical is chemically added to the benzene-1,2-diamine to form an imine intermediate. The intermediary then undergoes (H_2O loss) so that the furan-linked benzimidazole derivative is formed. The effective overlap between the absorption band of Eosin Y and the emission spectrum of green LEDs enhances photon absorption relative to red LED irradiation, leading to faster reaction kinetics and higher product yield.

C. Product Characterization

Column chromatography was used to purify the product, and mass spectrometry (MS), 1H NMR, and ^{13}C NMR were used to characterize it.

- The presence of both structural pieces was confirmed by the 1H NMR spectra, which showed signals corresponding to the benzimidazole ring protons (δ 7.00–8.50 ppm) and aromatic protons of the 2-(furan-2-yl)-1H-benzimidazole moiety (δ 7.50–7.65 ppm).
- The creation of an amide-linked framework was consistent with the ^{13}C NMR spectrum, which had distinctive resonances at δ 152 ppm (C-C) and δ 143.8 ppm (C-N of benzimidazole).
- The successful synthesis of the product was confirmed by the mass spectrum (ESI-MS), which showed a molecular ion peak that matched the benzimidazole derivative's expected molecular weight.

Taken as a whole, these spectroscopic results clearly demonstrated that the furan-linked benzimidazole-based heterocyclic molecule was synthesised via a metal-free, green-light-mediated photo-redox process.

D. Comparative Analysis and Green Chemistry Aspects

- The current green LED photo redox method shows notable advantages over traditional thermal synthesis:
- Eosin Y was optimally excited under green light, resulting in a higher yield (82%).
- The reaction proceeds easily in mild, energy-saving settings at normal room temperature.
- Compared to standard reflux procedures, the response period is lower (70 minutes).
- Metal-free and sustainable, reducing the production of toxic waste.
- Good atom efficiency that aligns with the twelve principles of green chemistry.

This work demonstrates the efficiency of visible-light photo-redox catalysis using green LED irradiation as a sustainable, high-yielding method for the synthesis of bioactive benzimidazole compounds.

i. Overview of Result

The increased photochemical method using Eosin (Y) (1 mol%) in THF at ambient temperature and green LED light (18 W) is an efficient, repeatable, and sustainable method for producing furan-bonded benzimidazole compounds. The greater yield and selectivity achieved under green-light irradiation highlight the importance of matching photon energy to photocatalyst absorption to improve photo-redox efficiency. This process is more environmentally friendly than conventional heating and red-light-induced methods for forming heterocyclic compounds.

Table I: Improved Reactive Parameters

| Entry | Photocatalyst | Catalyst (mol%) | LED (18W) | Solvent | Time (min.) | Yield (%) |
|-------|---------------|-----------------|-----------|---------|-------------|-----------|
| 1 | Eosin-Y | 1 | Green | THF | 70 | 82 |
| 2 | Eosin-Y | 1 | Blue | THF | 80 | 79 |
| 3 | Eosin-Y | 1 | Red | THF | 90 | 76 |
| 4 | Rose Bengal | 1 | Green | THF | 90 | 77 |
| 5 | Rose Bengal | 1 | Blue | THF | 90 | 81 |
| 6 | Rose Bengal | 1 | Red | THF | 90 | 78 |
| 7 | Rhodamine B | 1 | Green | THF | 90 | 71 |
| 8 | Rhodamine B | 1 | Blue | THF | 90 | 67 |
| 9 | Rhodamine B | 1 | Red | THF | 100 | 81.5 |

ii. Optimization of Reaction Conditions

The photocatalyst, solvent, light source, and reaction time were varied to optimise the reaction parameters (Table I).

After 70 minutes at ambient temperature, Eosin Y performed best under green LED radiation ($\lambda = 530$ nm, 18 W) among the dyes

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examined: Eosin Y, Rose Bengal, and Rhodamine B. As a result, the required benzimidazole derivative was obtained in the highest yield (82% in 70 min).

Reactions using various colours or solvents, such as ethanol, acetonitrile, and dichloromethane, yielded lower yields. The fact that the reaction ceased in the absence of either light or the photocatalyst demonstrated the essential roles of each. Eosin Y (1 mol%), THF (10 mL), a green LED (18 W), and 70 minutes of room-temperature irradiation were found to be the optimal conditions for achieving the highest yield of the required benzimidazole derivative. 2-(furan-2-yl)-1H-benzimidazole analysis. Under optimal visible-light (green LED) conditions, the synthesised chemical 2-(furan-2-yl)-1H-benzimidazole formed as a yellow crystalline solid in good yield.

iii. *Physical Data*

M. F.: C₁₁H₈N₂O, crystalline solid, white to off-white, Melting Point: 250 °C (uncorrected), M.W:184.12 g/ml, Rf value (TLC):0.55- 0.65: Observed on silica gel using Benzene: Ethanol (8:2), Yield (isolated): 82%, Eosin Y (1 mol%), THF (10 mL), Green LED ($\lambda = 535$ nm, 18 W), 70min.

iv. *Testing Session*

Visible-Light Photo Redox Synthesis of Analogues of Benzimidazoles



Eosin-Y, THF, Rt 70 min. Visible Light(Green LED)

¹H NMR (400 MHz, DMSO-d₆): δ 12.12 (bs, 1H, –NH), 7.50-7.60 ppm (m, 2H), 7.0-7.2 ppm (m, 2H), 7.85-7.90 ppm (dd, J = 1.7, Hz, J = 0.8 Hz, 1H), 7.20-7.21 ppm (d, J = 3.2 Hz or 4.0 Hz, 1H), 6.5-6.7 ppm (dd, J = 3.1 Hz, J = 1.7 Hz, 1H)

¹³C NMR (400 MHz, DMSO-d₆): δ 152.0, 142.6, 143.7, 141.5, 131.8, 121.6, 117.5, 111.8, and 110.4 ppm.

ESI-MS(m/z): 184 M⁺ ([M+H])⁺base peak, 183, 155, 128, 102, 77



[Fig.1: GA1]

Furan-link benzimidazole derivatives are produced in THF under green LED irradiation (535 nm) at room temperature using visible light, Eosin Y catalytic reaction, with no metal. Using a SET mechanism, the reaction yields 82% of the substance over 70 minutes. (Figure 1 GA1)

E. Mechanistic Consideration

Under green LED irradiation, eosin Y absorbs visible photons and is promoted to its excited singlet state (¹EY*), which undergoes intersystem crossing to generate the triplet excited state (³EY*). This excited dye acts as a single-electron transfer (SET) catalyst, facilitating electron transfer between

the substrate and the photosensitizer. In this reaction, eosin Y accepts an electron from furfural, forming a radical that then reacts with benzene 1,2-diamine to yield the desired linked benzimidazole after water removal. The whole process occurs under conditions without any extra heat or special atmosphere, which shows how simple and environmentally friendly this photo redox method is.

F. Comparison with Traditional Methods

This way of making benzimidazole with light is really good because it offers many advantages over older methods that use heat or metal. The old ways usually need helpers like copper, zinc or aluminium oxide to make the reaction work. The visible-light method is superior to the thermal or metal-catalysed benzimidazole syntheses.

- i. *This Method Works Without Metal:* it gets rid of the need, for dangerous catalysts.
- ii. *It Works Well in Conditions:* the reaction happens easily in visible light at room temperature.
- iii. *Eco-Friendly Materials:* Eosin Y is cost-effective, safe, and compatible with solvents, which are good for the environment.
- iv. Waste and the creation of byproducts remain unchanged by the use of strong reagents or external oxidants.

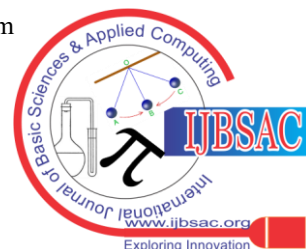
G. Yield and Purity Evaluation

The improved light-redox reaction with a green LED ($\lambda = 535$ nm) produced 2-(furan-2-yl)-1H-benzimidazole in 82% yield, compared to previously described photo-redox methods (typically 70–85%). Using column chromatography, a pure product with an Rf value of 0.55 to 0.65 was obtained (benzene: ethanol, 8:2). The crystalline solid and bright TLC spots suggest high purity and efficient conversion with few side products.

H. Spectroscopic Characterization

- i. **IR**
- ii. 2827 – 2630: Broad stretching for the N-H bond (benzimidazole ring).
- iii. 1600 – 1560: Stretching vibrations for aromatic C=C and C=N bonds.
- iv. 1540 – 1417: Asymmetric and symmetric ring stretching.
- v. 1367 – 1095: Furan ring breathing and C-H in-plane bending.
- vi. 850 – 730: C-H out-of-plane bending and furan ring deformation.
- vii. ¹H NMR (400 MHz, DMSO-d₆): δ 12.12 (bs, 1H, –NH), 7.50-7.60 ppm (m, 2H), 7.0-7.2 ppm (m, 2H), 7.85-7.90 ppm (dd, J = 1.8, Hz, J = 0.9 Hz, 1H), 7.20-7.21 ppm (d, J = 3.3 Hz or 4.0 Hz, 1H), 6.5-6.7 ppm (dd, J = 3.3 Hz, J = 1.8 Hz, 1H)
- viii. ¹³C NMR (400 MHz, DMSO-d₆): δ 152.0, 142.6, 140.7, 143.5, 131.8, 121.6, 118.5, 111.8, and 110.5 ppm.
- ix. ESI-MS(m/z): 184 M⁺ ([M+H])⁺base peak, 183, 155, 129, 103, 77

The spectroscopic data confirm the structure and purity of the synthesised compound.





I. Comparative and Literature Context

Previous photo-redox techniques employing Ru(bpy)₃²⁺ or Ir(ppy)₃ catalysts typically required controlled, inert conditions and yielded lower yields. In contrast, exposure of Eosin Y to green LED light achieves comparable or superior reactivity within a sustainable, metal-free system. Furthermore, the resulting product structure aligns with established bioactive benzimidazole scaffolds, suggesting potential pharmacological relevance and enabling earlier biological evaluation.

IV. CONCLUSION

In summary, a green, successful, and metal-free method for the production of benzimidazole derivatives via visible-light-induced photo-redox catalysis has been developed using Eosin Y under green LED irradiation. The reaction proceeds readily at room temperature, producing the required furan-linked derivative in high yield and purity. The structure of the synthetic heterocycle was verified by spectroscopy (IR, NMR, and MS). This eco-friendly method reduces waste and energy consumption while providing a practical basis for the synthesis of biologically active benzimidazole derivatives with potential antifungal properties.

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DECLARATION STATEMENT

After aggregating input from all authors, I must verify the accuracy of the following information as the article's author.

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- **Ethical Approval and Consent to Participate:** The content of this article does not necessitate ethical approval or consent to participate with supporting documentation.
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- **Author's Contributions:** The authorship of this article is contributed equally to all participating individuals.

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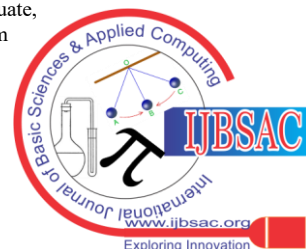


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