

## Novel D- $\pi$ -A Iminocoumarin-Based Molecules: Synthesis, Photophysical Properties, and Preliminary Evaluation as Photosensitizers for DSSCs

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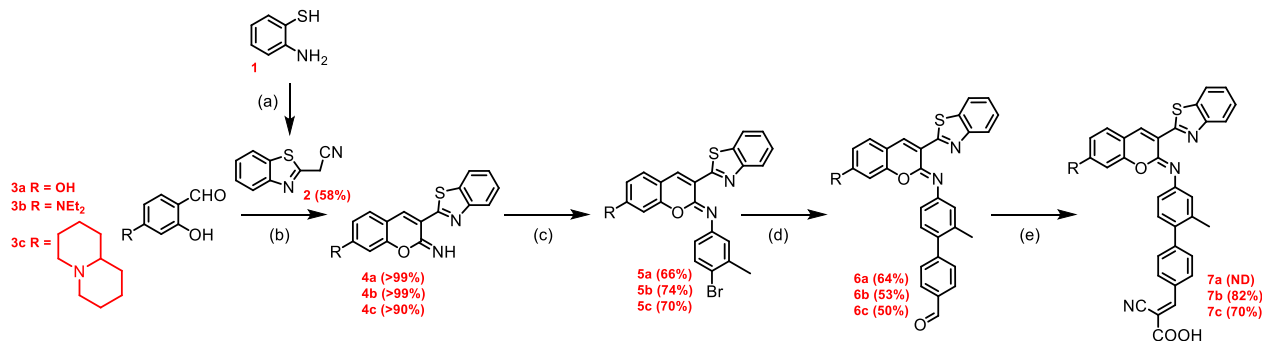
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### ABSTRACT

In recent years, coumarin derivatives have generated significant interest in their applications in dye-sensitized solar cells (DSSCs) due to the ease of modifying their photophysical properties by introducing substituents/groups. Thus, the present work reports the synthesis of iminocoumarin benzothiazole hybrids to investigate their potential applications as sensitizers in DSSCs (Scheme 1). Initially, 2-aminothiophenol (**1**) underwent a cyclization reaction with malonitrile in ethanol and acetic acid, yielding benzothiazole **2**. Subsequently, **2** underwent a Knoevenagel condensation reaction with hydroxybenzaldehyde (**3**) in the presence of piperidine and ethanol, resulting in iminocoumarins **4**. The reaction of **4** with 4-bromo-3-methylaniline produced the desired intermediates, 2-phenyliminocoumarins **5**. These intermediates underwent a Suzuki coupling reaction with 4-formylphenylboronic acid to form **6**. Finally, the condensation reaction between **6** and cyanoacetic acid, led to photosensitizers **7** in good yields (70-82%). The structures of the synthesized target compounds were characterized by FTIR, <sup>1</sup>H-NMR, HRMS, and UV-Vis spectra. Therefore, preliminary results show that the target compounds can be considered precursors for the design of coumarin-based D- $\pi$ -A molecules and can be used in further studies.



**Scheme 1.** Synthesis of iminocoumarin-benzothiazole hybrids. Reagents and solvents: a) malonitrile, EtOH, AcOH; b) EtOH, piperidine; c) 4-bromo-3-methylaniline, AcOH; d) 4-formylphenylboronic acid, K<sub>2</sub>CO<sub>3</sub>(aq), THF, Pd(PPh<sub>3</sub>)<sub>4</sub>; e) NCCH<sub>2</sub>COOH, piperidine, ACN.

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