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Preparation of Allyl BODIPY for the Click Reaction with Thioglycolic Acid

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Abstract : Photodynamic therapy (PDT) is currently used for the treatment of malignancies and premalignant tumors. It is based on the capture of a photosensitizing molecule (PS) which, when excited by light at a certain wavelength, reacts with oxygen and generates oxidizing species (radicals, singlet oxygen, triplet species) in target tissues, leading to cell death. BODIPY (4,4-difluoro-4-bora-3a,4a-diaza-s-indaceno) derivatives are emerging as important candidates for photosensitizer in photodynamic therapy of cancer cells due to their high triplet quantum yield. Today these dyes are relevant molecules in photovoltaic materials and fluorescent sensors. In this study, it will be demonstrated the possibility that BODIPY can be covalently linked to thioglycolic acid through the click reaction. Thiol−ene click chemistry has become a powerful synthesis method in materials science and surface modification. The design of biobased allyl-terminated precursors with high renewable carbon content for the construction of the thiol-ene polymer networks is essential for sustainable development and green chemistry. The work aims to synthesize the BODIPY (10-(4-(allyloxy) phenyl)-2,8-diethyl-5,5-difluoro-1,3,7,9-tetramethyl-5H-dipyrrolo[1,2-c:2',1'-f] [1,3,2] diazaborinin-4-ium-5-uide) and to click reaction with Thioglycolic acid. BODIPY was synthesized by the condensation reaction between aldehyde and pyrrole in dichloromethane, followed by in situ complexation with BF3·OEt2 in the presence of the base. Then it was functionalized with allyl bromide to achieve the double bond and thus be able to carry out the click reaction. The thiol−ene click was performed using DMPA (2,2-Dimethoxy-2-phenylacetophenone) as a photo-initiator in the presence of UV light (320–500 nm) in DMF at room temperature for 24 hours. Compounds were characterized by standard analytical techniques, including UV-Vis Spectroscopy, 1H, 13C, 19F NMR and mass spectroscopy. The results of this study will be important to link BODIPY to polymers through the thiol group offering a diversity of applications and functionalization. This new molecule can be tested as third-generation photosensitizers, in which the dye is targeted by antibodies or nanocarriers by cells, mainly in cancer cells, PDT and Photodynamic Antimicrobial Chemotherapy (PACT). According to our studies, it was possible to visualize a click reaction between allyl BODIPY and thioglycolic acid. Our team will also test the reaction with other thiol groups for comparison. Further, we will do the click reaction of BODIPY with a natural polymer linked with a thiol group. The results of the above compounds will be tested in PDT assays on various lung cancer cell lines.

Keywords : bodipy, click reaction, thioglycolic acid, allyl, thiol-ene click
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