



Detail Synthetic Study of Infrared Fluorescent Dyes: Design, Synthesis and Chemical Properties of their Photodynamic Therapy Probes

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ARTICLE INFO

Article history:

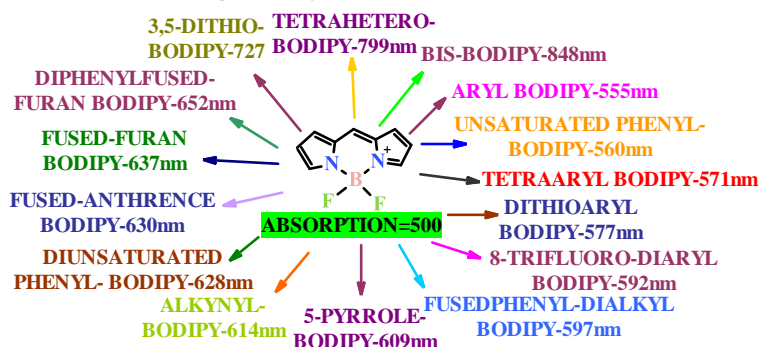
Received
Received in revised form
Accepted
Available online

Keywords:

BODIPY
Photodynamic Therapy
Biological Probes
Photosensitizers
Fluorescence
QSAR-Studies

ABSTRACT

Dipyromethene boron difluoride (BODIPY) derivatives can be used as effective photosensitizers (PS's) to eradicate a broad spectrum of microbes that threaten the global population health. Moreover, these compounds could be used in diagnostic or therapy, controlling the balance between the fluorescence emission and the photodynamic activity. There is still much work to be done in the search for ideal PS's with applications in photodynamic therapy (PDT). To effectively use near infrared region BODIPY dyes for labelling during biological analyses, or as biomarkers in biomedical applications such as imaging diagnosis, a hydrophilic character is usually required. It was found that the introduction of the strong electron-withdrawing group at the *meso* position in the BODIPY skeleton was responsible for the drastic bathochromic shift in the absorption spectrum. Several studies on the development of small molecule fluorescent probes have been performed with short wavelengths and with poor water solubility. There should be new investigations to obtain more information on the mechanisms of photodynamic action relating to cell damage and experiments in vivo infection models. In order to understand the effect of the substituents, a predictive quantitative structure-activity relationship (QSAR) regression model, based on theoretical holistic molecular descriptors as developed. An even better fluorescent probe would combine the photostability of the BODIPY group with a chromophore that absorbs at longer wavelength that makes for better light penetration in cells and tissues. In this review, we will summarize ideas on different wavelengths and hydroelectric abilities through modifications of molecular structures of the biological probe molecule. BODIPY's materials and chemical modification methods for modulating the optical properties presented here could be versatile for developing efficient photo-responsive bio-related materials to control the biological activities and efficient quenchers on the biotechnological assays with labelled biomolecules.



ABBREVIATION: BODIPY: 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene, PS: photosensitizers, PDT: photodynamic therapy, QSAR: quantitative structure-activity relationship, NIR: Near-Infrared, ROS: Reactive Oxygen Species, DNA: DeoxyriboNucleic Acid, CRC: aggregation-caused

fluorescence quenching, TFA: Tri Fluoroacetic Acid, PET: Photo Electron Transfer, EDG: Electron Donating Groups, HOMO: Highest Occupied Molecular Orbital, LUMO: Lowest Unoccupied Molecular Orbital, BCOD: bicyclo[2.2.2]octadiene, AIE: aggregation-induced emission, TICT: twisted

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