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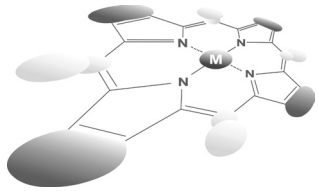

Synthesis and photophysicochemical properties of BODIPY dye functionalized gold nanorods for use in antimicrobial photodynamic therapy

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Dedicated to Professor Tomás Torres on the occasion of his 65th birthday

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ABSTRACT: A series of boron dipyrromethene (BODIPY) dyes with properties that are ideal for a good photosensitizer have been prepared. Functionalization with bromine atoms and attachment to gold nanoparticles through a *meso*-aniline group results in high singlet oxygen quantum yields and low fluorescent quantum yields. Molecular modelling was used to analyze trends in the MO energies of various brominated aniline BODIPY dyes.

KEYWORDS: BODIPY, singlet oxygen, XPS spectroscopy, TD-DFT calculations, APDT.

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INTRODUCTION

In recent years, bacterial resistance to conventional antibiotics has increased significantly, so there is a pressing need for alternative treatments [1]. Antimicrobial photodynamic therapy (APDT) has proven to be one of the most promising alternatives for microbial control [2]. APDT follows similar principles to those of photodynamic therapy (PDT) for the treatment of cancerous cells, since it involves the eradication of target cells by reactive oxygen species, such as singlet oxygen, $^1O_2$ is produced by the interaction of a chemical photosensitizer (PS) with incident laser light of appropriate wavelength (ideally at the maximum absorption wavelength of the PS) [3]. Bacterial resistance to APDT is highly improbable [4–6], since bacteria are inactivated by the $^1O_2$ and other reactive species. A good PS possesses the ability to strongly absorb incident laser light, with efficient intersystem crossing to the triplet state, and then energy transfer to molecular oxygen. Dyes possessing such characteristics are typically rigid planar structures possessing a high degree of π-conjugation [7]. Macrocyclic photosensitizers such as porphyrins and phthalocyanines have been widely used for APDT [7–9]. There are some major drawbacks associated with their use in biomedical applications, however, such as their lack of solubility in aqueous solvents and tumor specificity [10].

In recent years, boron dipyrromethene (BODIPY) have been evaluated as an alternative to these dyes, to provide a new class of potent PDT agents, because of their high molar absorption coefficient and photostability. Until recently, their strong absorption in the 500–550 nm region, high fluorescent quantum yields, negligible intersystem crossing to the triplet state and hence low production of singlet oxygen [11] had limited the interest in BODIPY dyes for singlet oxygen applications in biomedical research. The absence of absorption in the therapeutic window between 650–1000 nm hinders penetration of light to deep seated tumor cells. However, in recent years studies have shown that increasing π-conjugation through styrl, aryl and ethynylaryl substitution at the 1-, 3-, 5-, and/or 7-positions, aromatic ring fusion, or replacing the *meso*-carbon atom with an aza-nitrogen atom to form an aza-BODIPY dye, or a combination thereof can significantly shift the absorption band to higher wavelength [12]. It has been demonstrated that

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