Synthesis and Characterization of different BODIPY molecules, photophysical and computational studies

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Abstract

BODIPY dyes are widely studied for their exceptional photostability, tunable fluorescence, and diverse applications in imaging, sensing, and optoelectronics. These molecules are known to have a low Stokes shift, narrow absorption and emission bands, high fluorescence quantum yields, and excellent photostability. Such features provide significant advantages compared to other organic fluorophores, making BODIPYs ideal candidates for both fundamental research and applied sciences. These properties make them interesting for photodynamic therapy, cellular imaging, drug delivery, and also as organic photovoltaic materials. [1,2] In addition, their chemical versatility enables structural modifications that allow fine-tuning of electronic properties, solubility, and biocompatibility, which is highly desirable for interdisciplinary applications.

In this study, a series of thirteen BODIPY derivatives (Fig.1) bearing varied meso-substituents were synthesized and thoroughly characterized. Structural analysis was performed using protonic, carbon, and fluor NMR, mass spectrometry, and IR spectroscopy, while UV-Vis and fluorescence spectroscopy revealed that meso-substitution significantly influences the optical properties, particularly fluorescence quantum yields and spectral profiles. These experimental results provide a deeper understanding of how subtle structural variations directly impact photophysical behavior.

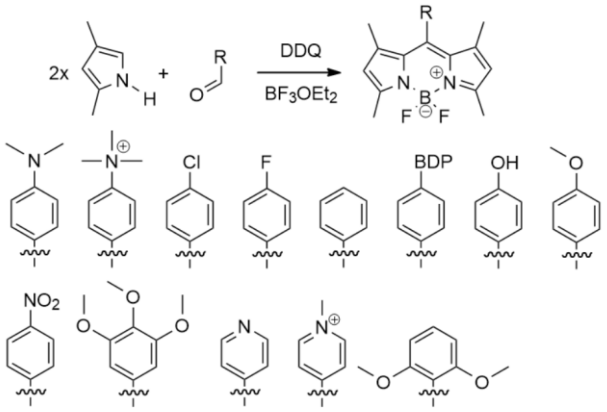

Fig.1 – Structure and general synthetic path of 13 BODIPY derivates

Complementary computational studies, including HOMO–LUMO energy gap analysis, oscillator strengths, and TD-DFT calculations, supported the experimental observations. The correlation between theoretical predictions and measured spectra demonstrates the reliability of computational methods for guiding the rational design of new derivatives. These findings offer valuable insights into structure–property relationships in meso-substituted BODIPYs and underscore their potential for fluorescence-based technologies. Preliminary studies were also conducted using Saponite for the synthesis of hybrid materials, in order to better understand the interaction between the chosen BODIPY dyes and 2D clay minerals. Such hybrid systems may open up opportunities for the development of functional nanomaterials, catalysis, and advanced sensing platforms.

(1) “BODIPY Dyes and Their Derivatives: Syntheses and Spectroscopic Properties”, A. Loudet and K. Burgess, Chemical Reviews, Vol. 107 (2007) 4891-4932.
(2) “The chemistry of fluorescent bodipy dyes: versatility unsurpassed”, Ulrich G, Ziessel R, Harriman A. Angewandte Chemie International Edition, Vol. 47 (2008) 1184-1201.