

# Synthesis and characterization of a BODIPY dimer for photodynamic therapy



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#### INTRODUCTION

Since their discovery in 1964, the BODIPYs present themselves as an important line of research in chemistry, biochemistry, medicine, sensors and alternative energies, confirming the BODIPY as a relevant organic class of compounds with a wide range of applications [1-3]. In this work we studied the synthesis and characterization of a BODIPY dimer through photophysical studies in order to evaluate its purity and yield of reaction and its possible use in Photodynamic Therapy.

## RESULTS



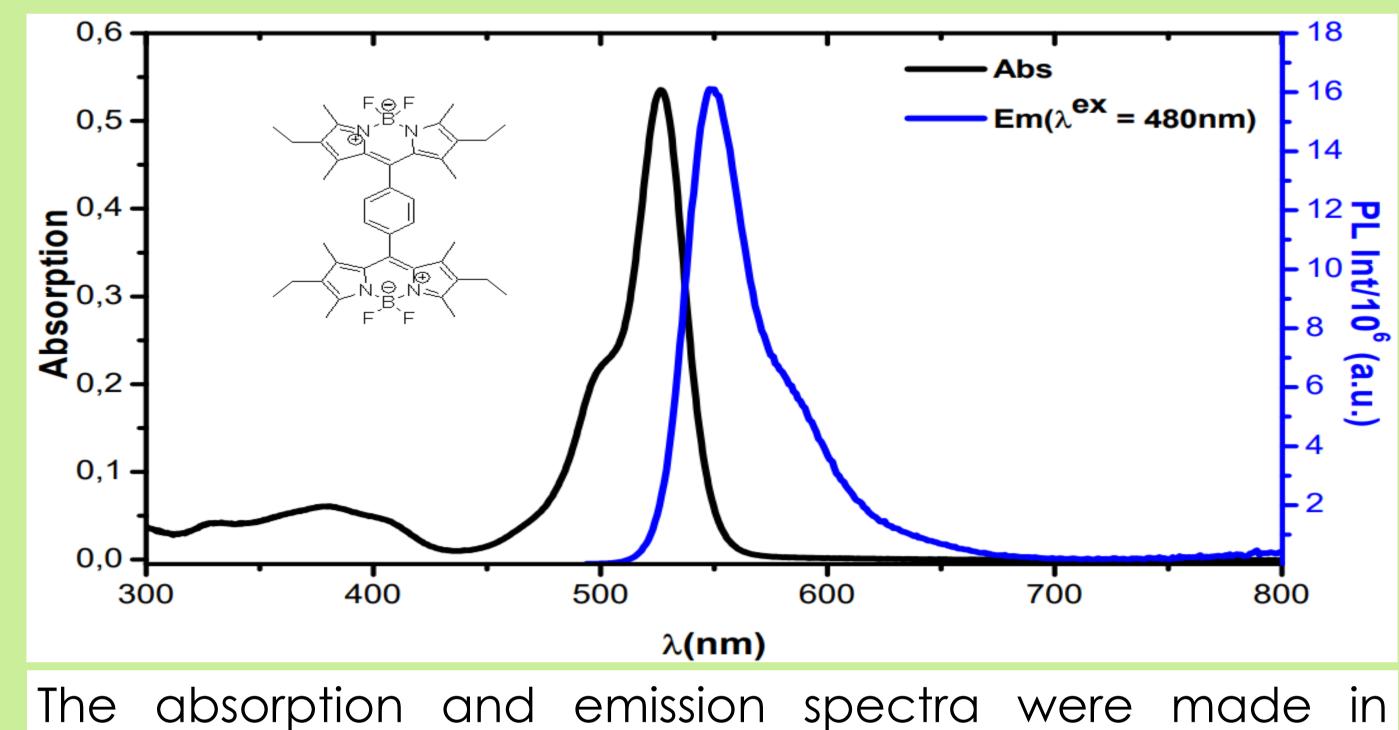
Our BODIPY dimer presents a strong colour concentration dependence demonstrating different colours at different concentrations of the dimer under UV light (right) and normal light (left) with dichloromethane/hexane (6/4) as a solvent.

#### **OBJECTIVES**

The objective of this work was to synthetize a BODIPY phenyl dimer, characterise it and make photophysical studies with the dimer, all this to determine its potential applications in medical studies of cancer therapy, namely on the Photodynamic Therapy of cancer.

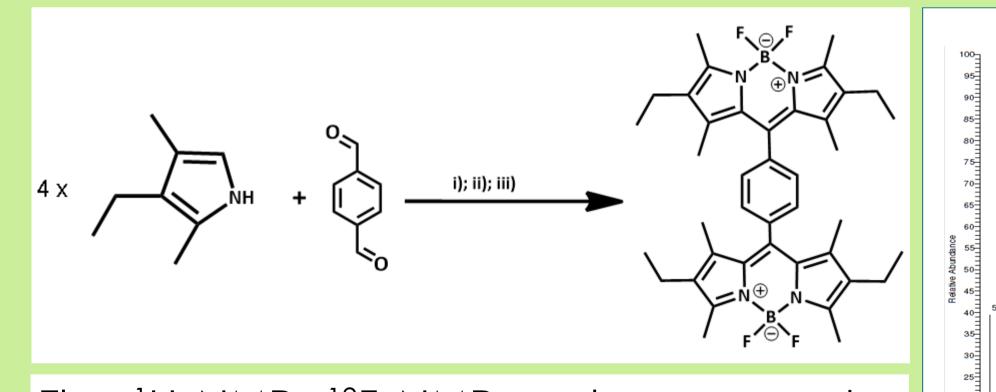
**MATERIALS AND METHODS** 

General procedure for the preparation of the BODIPY 10,10'-(1,4-fenilene)bis(2,8-dietil-5,5-difluoro-1,3,7,9-tetrametil-5H-dipirrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide): i)TFA; ii)DDQ; iii)diisopropylethylamine,  $BF_3.O(C_2H_5)_2$ .

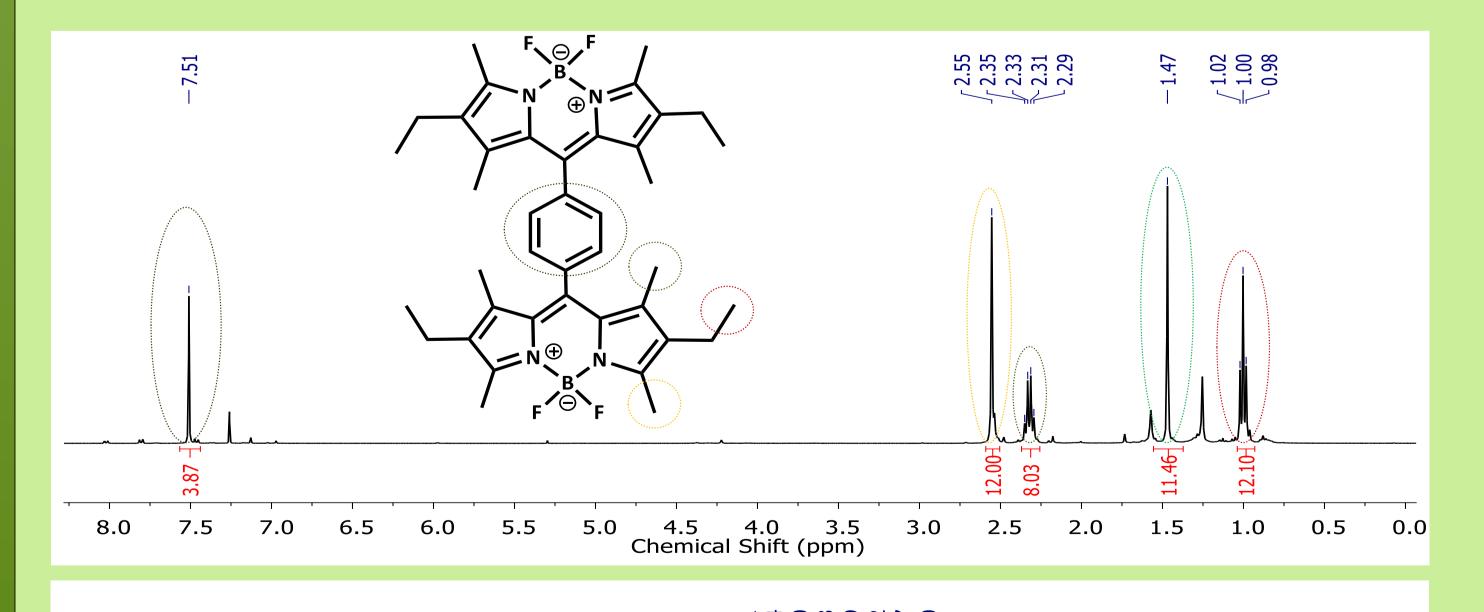


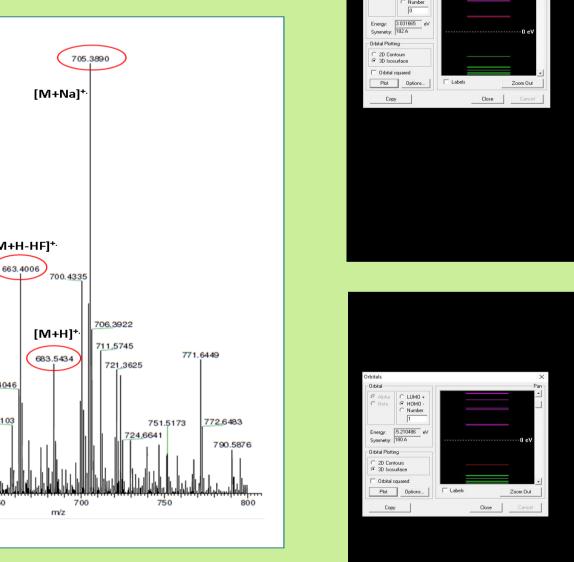
toluene at room temperature.



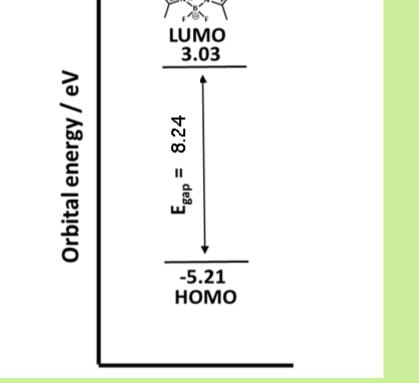


The <sup>1</sup>H NMR, <sup>19</sup>F NMR and mass spectra confirm the structure of the BODIPY dimer.



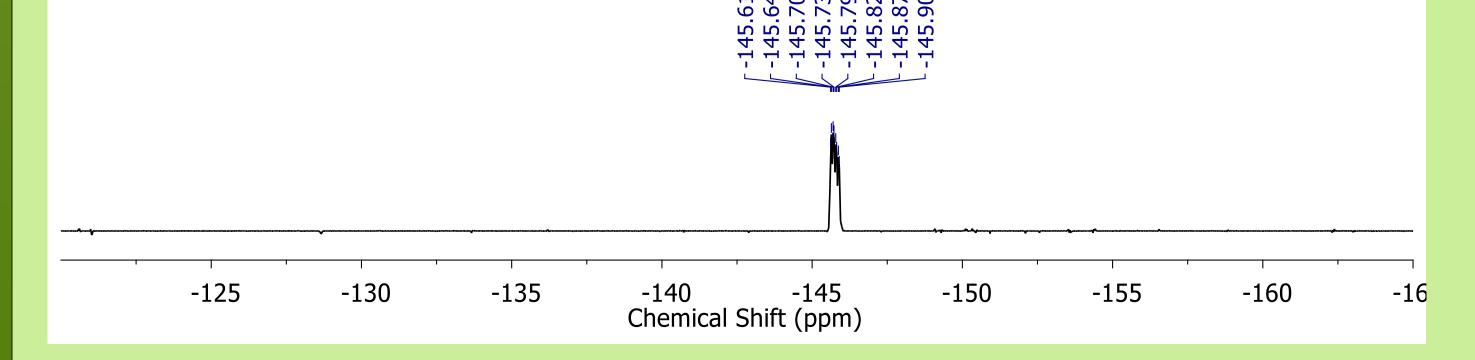


### CONCLUSION



HOMO (-5.21 eV) and LUMO (3.03 eV) Calculations *ab initio* in Hyperchem with Minimal Basis Set (STO-3G) with (HyperGauss with 298 basis functions and 894 primitive gaussians). Geometry minimization with a Polak-Ribiere algoritm with a RMS of 0.5 kcal/(A mol).

The BODIPY dimer with a *meso* phenyl linker was synthesized and characterized. Our studies show a good separation HOMO LUMO and an intense absorption and fluorescence spectra that allow us to advance to the next phase of biocompatibility studies prior to the PDT assays.



#### REFERENCES

 "BODIPY Dyes and Their Derivatives: Syntheses and Spectroscopic Properties", A. Loudet and K. Burgess, Chemical Reviews, Vol. 107 (2007) 4891-4932.
"The chemistry of fluorescent bodipy dyes: versatility unsurpassed", Ulrich G, Ziessel R, Harriman A. Angewandte Chemie International Edition, Vol. 47 (2008) 1184-1201.
"Synthesis, characterization and application of meso-substituted fluorinated boron dipyrromethenes (BODIPYs) with different styryl groups in organic photovoltaic cells", António Aguiar, Joana Farinhas, Wanderson da Silva, Mariana Emilia Ghica, Christopher M.A. Brett, Jorge Morgado, Abílio J.F.N. Sobral, Dyes and Pigments Vol. 168 (2019) 103-110.

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