A Water-Soluble Molecular Sensitizer for Solar Devices

Joshua Topley – 140644074 - J.Topley1@Newcastle.ac.uk - Mchem with Hons in Chemistry
Supervised by Dr Fabio Cucinotta

Newcastle University

AIMS

- To use the methods of J. G. Wang, et al[1] and B. Brizet, et al[2] to develop a new synthetic method for the production of a boron-dipyrromethene type dye with improved light absorbance and water solubility characteristics.
- To characterise the target molecule using analytical techniques such as UV-Vis spectroscopy which analyses the absorbance of ultra-violet and visible light to determine the effectiveness of the target molecule as a light absorbing compound.
- To incorporate the target molecule into a solar cell device to test efficiency of the molecule for potential use in solar cell devices.

Introduction

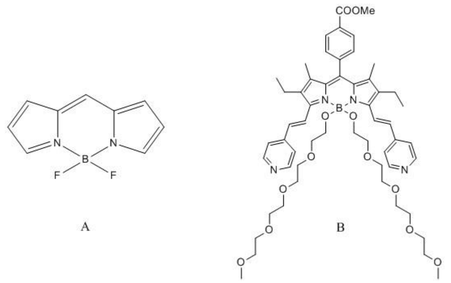

***Figure 1**. A: Common BODIPY unit consisting of dipyrromethene complexed to BF_2 B: Target molecule to be produced with extended functionalisation of core BODIPY structure to improve light absorbance and water solubility characteristics of the molecule.*

Dye sensitised solar cells are a form of 3rd generation solar cell technology that relies on an organic dye as the light absorbent material. Dye sensitised cells have the advantage of being thinner, lighter, cheaper and easier to produced than silicon based solar cells seen on the rooftops of houses today. The organic dyes used in such cells determine the efficiency of the cell in producing energy from light, therefore research into producing new organic dyes is of high importance in the area. Boron-dipyrromethene (BODIPY) dyes are a class of fluorescent dyes, commonly used as light absorbent materials due to their good light absorption characteristics and their conjugated systems which make them ideal charge carriers. BODIPY dyes are characterised by the presence of dipyrromethene complexed with a disubstituted boron atom, usually BF_2, this common unit is shown as complex A in figure 1. The objective of this research was to take the common BODIPY structure and add additional functional groups to it in order to produce a BODIPY dye with increased solar absorption characteristics and improved water solubility which would improve the efficiency of dye solar cells and the ease of their production respectively.

Method

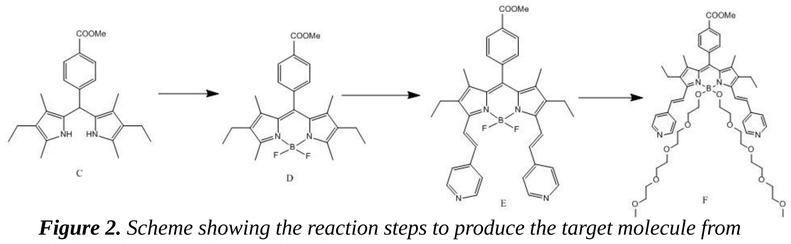

***Figure 2.** Scheme showing the reaction steps to produce the target molecule from the base dipyrromethene molecule.*

In order to produce the target molecule the reaction scheme shown in figure 2, was developed from the literature[1][2] although changes were made to the conditions given by J. G. Wang, et al[1] in order to account for the chemicals available for this work. Initially compound C was produced by combining a 2 equivalents of a tri-substituted pyrrole and 1 equivalent of the phenyl aldehyde in water under a nitrogen atmosphere. The dipyrromethene, C, produced was then purified before being oxidised using an oxidising agent overnight. Triethylamine and boron trifluoride diethyl etherate were then added to the oxidised dipyrromethene in order to produce the core BODIPY, D. Once this scheme of reaction was successfully completed, it was repeated on a larger scale to provide appropriate amounts of the core BODIPY for repeated further reactions to determine appropriate reaction conditions. The first functionalisation step required the core BODIPY to be heated at reflux (boiling the solution with a condenser which causes any evaporation to condensate and drip back into the reaction mixture.) in toluene in the presence of the functional group being added as well as glacial acetic acid and piperidine for 16 hours. After reflux the product could then be collected and purified. The final functionalisation required a short reflux of the BODIPY, E, with aluminium chloride for 20 minutes before adding 5 equivalents of the long chain functional group to the reaction mixture and stirring at room temperature for 2 hours. Once this has been completed the produced target material could be collected and purified for further testing.

Results

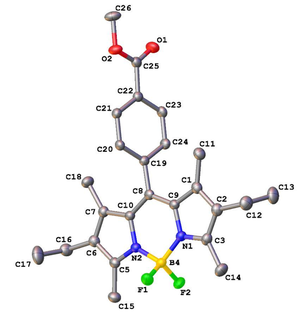

***Figure 3.** 3-dimensional structure of the successfully produced core BODIPY obtained using x-ray crystallography techniques.*

Initial reactions proceeded as expected with little difficulty producing the dipyrromethene, C, and the core BODIPY, D. A relatively high yield of around 30% on average was obtained for the synthesis of the BODIPY, D, which is comparable with similar reactions of this type. Purification of the molecules formed proved more difficult, time consuming column chromatography, in which chemicals are passed through a tube filled with silica at different rates depending on their affinity to the silica and solvent mixture used. Samples of good purity were obtained from column chromatography despite issues finding appropriate solvents in which the products would dissolve, however some yield was lost in the purification. Figure 3 above shows a 3-dimensional model of the core BODIPY, D, which was successfully produced however further functionalisation to form molecule E from figure 2 proved unsuccessful with reactions failing to proceed as expected leaving large amounts of starting material remaining at the end of the reaction which were difficult to extract from the reaction. Column chromatography was performed on the reaction mixture and nuclear magnetic resonance spectroscopy was used to identify the different materials extracted confirming the presence of starting materials remaining the reaction mixture after heating. Further reactions were preformed making adjustments to the ratios of starting materials, solvents and conditions used but none were successful.

Conclusions

As reaction conditions were changed from those used by J. G. Wang ,et al[1] further tests could be done using the reaction conditions as they were given in the literature as well as for different reaction conditions to understand why the particular reaction conditions used in this research failed to achieve the desired results. Once this barrier has been overcome research can continue as the scheme in figure 2 depicts and further functionalisation reactions can be attempted in order to produce the target molecule for characterisation and testing as per the original aims of this research.

Acknowledgments and References

I would like to thank Newcastle university and the school of chemistry for funding this research and Dr Fabio Cucinotta and Ben Jarman for their assistance in carrying out this research.

[1] - J. G. Wang, Y. J. Hou, W. H. Lei, Q. X. Zhou, C. Li, B. W. Zhang, and X. S. Wang, ChemPhysChem, 2012, 13, 2739 – 2747
[2] – B. Brizet, C. Bernhard, Y. Volkova, Y. Rousselin, P. D. Harvey, C. Goze, and F. Denat, Org. Biomol. Chem., 2013, 11, 7729