ESCULETIN-BASED ORGANIC CHROMOPHORES FOR DYE SENSITIZED SOLAR CELLS

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INTRODUCTION

The development of efficient solar energy harvesting systems is one of the greatest scientific challenges today. Recently attention has been driven to alternative solar collecting devices based on an optical absorbing chromophore anchored to the semiconductor surface. Our previous work on coumarins demonstrated that this molecules can be easily tune to incorporate substituents that allow to increase the conjugation at the 3-position.[1] In a completely new approach we developed new dye-sensitized solar cells, based on Grätzel's model. The optical absorbing chromophore was built on 6,7-dihydroxycoumarin (Esculetin, a natural product), a linker based on ethenylaryl substituents and at the end a strong electron acceptor moiety anchored to the semiconductor surface.

SYNTHESIS

The dyes **A**, **B** and **C**, are obtained in high yields, from the readily available 6,7-dihydroxy-coumarin (Figure 1).

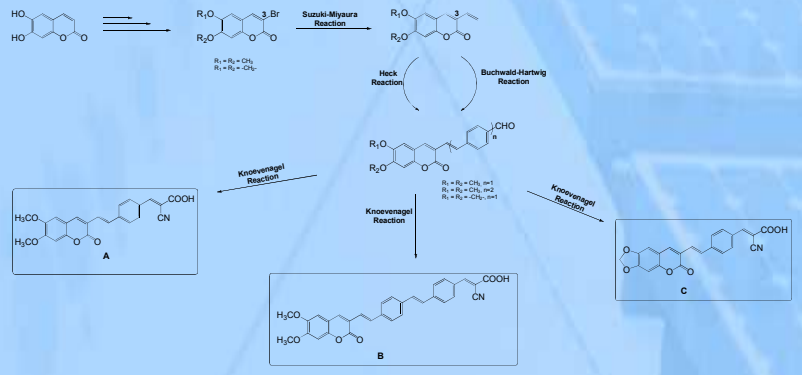

Figure 1 - Synthesis of 6,7-dihydroxycoumarin derivatives.

Photovoltaic Performance

At present, state-of-the-art DSSCs based on ruthenium(II)–polypyridyl complexes, e.g. N719 (Figure 2), as the active material have an overall power conversion efficiency (η) approaching 11% under standard illumination.[2]

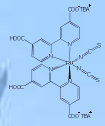

Figure 2 – Dye **N719**.
TBA⁺ = tetra-*n*-butylammonium

Evaluation of the dyes **A**, **B** and **C**, for solar-energy-to-electricity conversion (Figure 3, Table 1), allowed us to verify that the dye **A**, followed by **B,** showed the best performance, with an efficiency (*η*) of 1.37%, with a short-circuit current density (Jsc) of 3.36 mA cm^{-2}, an open-circuit voltage (Voc) of 0.59 V, and a fill factor of 0.69.[3]

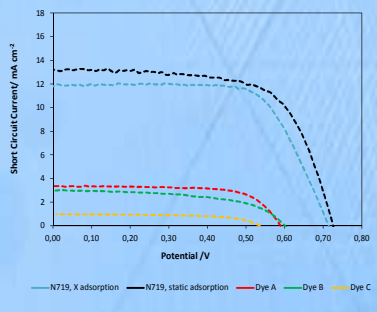

Figure 3 – Photocurrent intensity–voltage characteristics for the dyes **N719**, **A**, **B** and **C**.

Table 1 – Photovoltaic parameters for the dyes **N719**, **A**, **B** and **C** (short-circuit current density, Jsc ; open-circuit. voltage, Voc ; fill factor, FF and efficiency, η).

	N719, Static Adsorption	N719, Xadsoption	Dye A	Dye B	Dye C
Voc / V	0,73	0,71	0,59	0,60	0,54
Jsc / mA • cm^{-2}	13,14	11,82	3,36	2,98	1,00
MMP / mW • cm^{-2}	6,36	5,83	1,37	0,99	0,33
FF	0,66	0,69	0,69	0,55	0,62
η / %	6,36	5,83	1,37	0,99	0,33

Our results suggests that the structures **A** and **B,** whit a 6,7-dimethoxy system, are advantageous for effective electron injection from the dye into the conduction band of TiO_2, and the expansion of the π-conjugation by insertion of an additional styryl group, as in B (n=2) led to a decrease in efficiency probably due to the nonrigid bridging moiety, which causes energy losses by other photochemical.

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