Design, synthesis and characterization of novel thienylpyridazine derivatives for optical applications

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In recent years, push-pull π -conjugated systems bearing electron rich (thiophene, pyrrole, furan) and electron deficient heterocycles (pyridine, pyridazine, benzothiazole, etc.) have been widely used as NLO and photochromic materials, metal free organic sensitizers for DSSCs, OLEDs, etc. due to their easy synthesis and efficient tuning of the photophysical properties through small structural modifications.¹⁻²

During the last decade our research group has published experimental and theoretical results concerning the auxiliary donor/acceptor effect of electron rich and electron deficient heterocycles on π -conjugated systems.² Based on our earlier work we were motivated to extend these studies in order to explore the potential application of a new series of donor-acceptor substituted thienylpyridazines in which the pyridazine heterocycle plays the dual role of π -bridge and acceptor/auxiliary acceptor moiety. Therefore, the pyridazine ring was functionalized in position 3 with different (hetero)aryl-based groups (indole, benzonitrile and nitrophenyl) in order to study the effect of their electronic nature on the optical properties of the push-pull systems.

We report in this work the synthesis and the photophysical characterization of novel thienylpyridazine derivatives which were synthesized through Suzuki coupling of 3-bromo-6-(thiophen-2-*yl*)pyridazine³ with commercially available (hetero)aryl-boronic acids.

Keywords: push-pull π -conjugated systems, thiophene, pyridazine, Suzuki coupling, optical applications

Acknowledgements: Thank are due to *Fundação para a Ciência e Tecnologia* (Portugal) and FEDER-COMPETE for financial support through the Centro de Química PEst-C/QUI/UI0686/2011 (F-COMP-01-0124-FEDER-022716) and a PhD grant to S. S. M. Fernandes

(SFRH/BD/87786/2012). The NMR spectrometer Bruker Avance III 400 is part of the National NMR Network and was purchased with funds from FCT and FEDER.

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