A Comprehensive Investigation of Tryptanthrin Derivatives

Daniela Pinheiro¹*, Marta Pineiro¹, J. S. Seixas de Melo¹

¹ University of Coimbra, CQC, Department of Chemistry, Rua Larga, 3004-535, Coimbra, Portugal * dpinheiro@qui.uc.pt

Tryptanthrin (indolo[2,1-b]quinazoline-6,12-dione), abbreviated as TRYP, is a natural compound found in several natural sources that can also be synthetically obtained from indigo or isatin increasing the structural diversity of tryptanthrin derivatives.^{1,2} In the past recent years TRYP derivatives as well as its nanoformulations have been synthetized and evaluated for potential biological and pharmacological activity,³ and, very interesting, as stable active materials for all-organic redox flow batteries.⁴

In this work, halogenated tryptanthrins, amino and sulfonated tryptanthrin (*Figure 1*) were synthesized from indigo or isatin precursors. ^{1,2} Spectral and photophysical properties of the compounds, including quantitative determination of all the different deactivation pathways of S_1 and T_1 , were obtained in different solvents and temperatures.

The study of this set of tryptanthrin derivatives, including its singlet oxygen sensitization quantum yield clarify the interaction of this class of compounds with light, reveals its differences with indigo parents and open the way to their application as oxygen sensitizers.



Figure 1. Structures and acronyms of tryptanthrin (TRYP) and the studied derivatives.

Acknowledgements

D. Pinheiro acknowledge Coimbra Chemistry Centre (CQC) for the research grant UIDB/00313/2020 and Santander Universidades and University of Coimbra for the award "Projetos Semente de Investigação Científica Interdisciplinar Santander UC". The CQC is supported by the FCT, Portuguese Agency for Scientific Research, through the Projects UIDB/00313/2020 and UIDP/00313/2020. We also acknowledge the UC-NMR facility for obtaining the NMR data (www.nmrccc.uc.pt).

References

[1] D. Pinheiro, M. Pineiro, J. Pina, P. Brandão, A. M. Galvão. J. S. Seixas de Melo *Dyes Pigments* **2020**, 175, 108125.

[2] P. Brandão, D. Pinheiro, J. S. Seixas de Melo, M. Pineiro Dyes Pigments 2020, 173, 107935.

Iberian Symposium of Young Photochemists 2021

[3] R. Kaur, S. K. Manjal, R. K. Rawal and K. Kumar, *Bioorg. Med. Chem.*, 2017, 25, 4533-4552.
[4] D. Pinheiro, M. Pineiro, J. S. Seixas de Melo *Commun. Chem.* 2021, 4, 89.