

BRAZILIAN MEETING ON ORGANIC SYNTHESIS BENTO GONCALVES, RS - BRAZIL

Oxazoline-based dyes for fluorescent enantioselective differentiation of carbohydrates in solution

Natalí P. Debia,* Bruno B. de Araújo, Paulo F. B. Gonçalves, Fabiano S. Rodembusch, and Diogo S. Lüdtke

Instituto de Química, Universidade Federal do Rio Grande do Sul – UFRGS. Porto Alegre, RS, Brazil. *e-mail: <u>natali.debia@gmail.com</u>

Keywords: Chiral sensing, fluorescence spectroscopy, oxazoline

ABSTRACT

Understanding the interaction of small molecule with chiral biomolecules is key to study the mechanism of action of drugs in biological systems. As such, it is worth highlighting the enantiomeric differentiation of carbohydrate enantiomers in solution, applying a simple steady-state fluorescence emission spectroscopy. Herein, we present the synthesis of chiral 2-oxazolines derived from amino acids-based *N*-(2-hydroxyethyl) amides, containing a fluorophoric benzothiazole core. A series of six 2-oxazolines were synthetized in good yields and their photophysical properties were evaluated by UV-Vis absorption and fluorescence emission spectroscopies. Thereafter, these dyes were studied as optical sensors for the enantioselective differentiation of two carbohydrate enantiomers pairs in solution. Theoretical calculations have been performed to better understand the observed interaction dye-analyte. Results indicate that dye-bearing D-phenylalanine residue stands out exhibiting calculated enantioselectivity values higher than previously reported.¹ It is noteworthy that the obtained response is mainly due to weak interaction forces, such as hydrogen bonds.



ACKNOWLEDGEMENTS

Fundação de Amparo à Pesquisa do Rio Grande do Sul (FAPERGS), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and INCT-Catálise.

REFERENCES

¹ a) Debia, N. P.; Saraiva, M. T.; Martins, B. S.; Beal, R.; Goncalves, P. F. B.; Rodembusch, F. S.; Alves, D.; Lüdtke, D. S. *J. Org. Chem.* **2018**, *83*, 1348-1357; b) Debia, N. P.; Muller, J. M.; Gonçalves, P. F. B.; Rodembusch, F. S.; Lüdtke, D. S. *Spectrochim. Acta A* **2023**, 294, 122526.