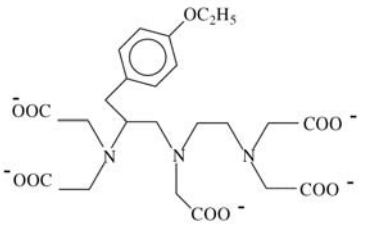
Study of the interaction of Ln^{3+} complexes of BOPTA or DPTA-Cholate with HSA and of DOTA/DTPA-Glycoconjugates with RCA_{120} using the High Resolution Saturation Transfer Difference (STD) NMR technique

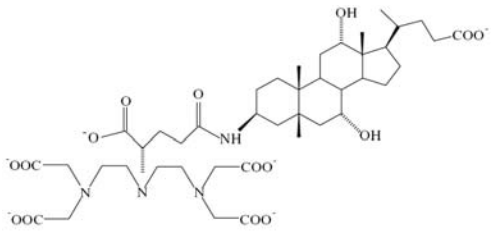
J. M. C. Teixeira[1,2] and C. F. G. C. Geraldes[1,2]

[1] Department of Biochemistry, Faculty of Science and Technology and [2]NMR Laboratory, Center of Neurosciences and Cell Biology, University of Coimbra, 3000 Coimbra, Portugal

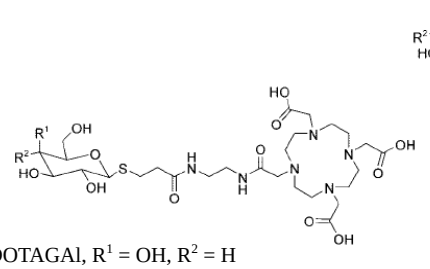
The study of ligand-receptor interactions using high resolution NMR techniques became much easier and with wider applications with the development of the Saturation Transfer Difference (STD) technique [1]. With such a protocol it is possible not only to rapidly determine if there is an interaction between a relatively small compound and a protein but also to screen out the ligand interaction specificity at atomic level, a characterization known as group epitope mapping (GEM). Our aim in this work is to prove the interaction between Gd^{3+}-based complexes, to be used as potential MRI contrast agents, with their supposed protein receptors and to characterize the ligand-protein binding interactions at an atomic level. We screened the interactions between the La^{3+} and Lu^{3+} complexes of BOPTA and DTPA-Cholate (B-22956/1) with Human Serum Albumin (HSA) [2] and between the La^{3+} and Lu^{3+} complexes of a group of DOTA-glyconjugates, namely DOTAGal, DOTALac, $DOTA(Lac)_2$ with the 120kDa lectin *Ricinus communis* agglutinin (RCA_{120}), used as a model for the asyaloglycoprotein receptor (ASGP-R)[3]. Our results were consistent with expectations based on previous literature [2,3]. They prove that LnDOTA-glyconjugates efficiently bind RCA_{120} through the galactose residue and also demonstrate that BOPTA and DPTA-Cholate complexes bind HSA through the aromatic ring and the cholic residue, respectively.



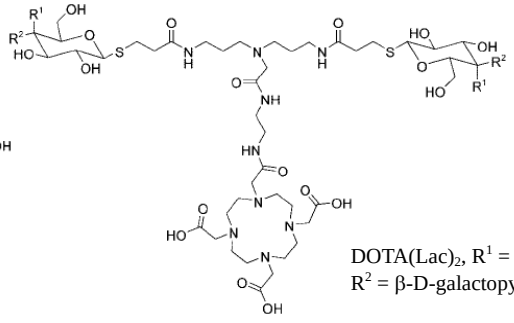
BOPTA



DPTA-Cholate



DOTAGAl, R^1 = OH, R^2 = H
DOTALac, R^1 = H, R^2 = β-D-galactopyranosyl



$DOTA(Lac)_2$, R^1 = H
R^2 = β-D-galactopyranosyl

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[2] Henrotte, V.; et. al., *J. Biol. Inorg. Chem.*, **2007**, *12*, 929-937.
[3] André, J. P.; Martins, J.A.; et al., *Chem. Eur. J.*, **2004**, *10*, 5804-5816;