CD STUDY OF THE IRON(II) CLATHROCHELATES WITH TERMINAL ALKYL CARBOXY OR SULFONYL GROUPS IN THE PRESENCE OF PROTEINS

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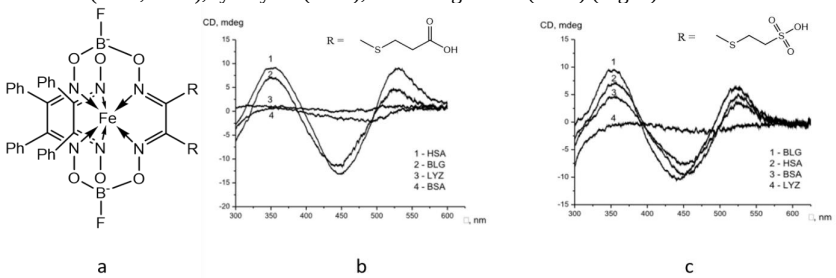
Clathrochelate complexes are the class of compounds that has shown a range of biologically active properties. Various studies show that nature of terminal ribbed functional groups is playing key role in its activity. In our recent study [1] we discovered that clathrochelate molecules bearing aryl carboxygroups form supramolecular complexes with serum albumins, in which inherently achiral clathrochelate molecule gives pronounced CD response. This occurs due to stabilization of the clathrochelate framework in one of selected chiral conformers in protein binding site and electrostatic interactions is very important for such binding. As continuation of this work we studied if exchange of terminal aryl carboxygroup to other types of functional ionizable groups make clathrochelate molecules CD sensitive to proteins. For this purpose, clathrochelates bearing alkyl carboxy and sulfo groups were synthesized and studied for their optical activity in presence of bovine and human serum albumins (BSA, HSA), lysozyme (LYZ), betalactogobulne (BLG) (Fig. 1).



a b c

Fig 1. The structure (a) and ICD-spectra of alkylcarboxy (b) and sulfoxygroup (c) terminated clathrochelates (c_{clt} = 20 μM) with different protein: BSA, HSA, LYZ and BLG ($c_{protein}$ = 40μM) in 0.05M Tris HCl, pH 7.9, 25 ^{0}C

The appearance of CD spectra of alkyl carboxy terminated clathrochelates shows that in order to fix one of the clathrochelate's conformation, the ribbed substituents bearing carboxygroup are not necessary to be rigid. The same goes for the sulfoxygroup which now is known to lead to formation of supramolecular complex as well.

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[1] V.B. Kovalska, S.V. Vakarov, M.V. Kuperman, M.Y. Losytskyy, E. Gumienna-Kontecka, Y.Z. Voloshin and O.A. Varzatskii, Induced chirality of cage metal complexes switched by their supramolecular and covalent binding, *Dalton Trans*, 2018, **47**, 1036-1052.