Dicarboxyl-terminated iron(II) clathrochelates as ICD-reporters for globular proteins.

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Streszczenie

Cage metal complexes iron(II) clathrochelates, which are inherently CD silent, were discovered to demonstrate intensive output in induced circular dichroism (ICD) spectra upon their assembly to albumins. With the aim to design clathrochelates as protein-sensitive CD reporters, the approach for the functionalization of one chelate α-dioximate fragment of the clathrochelate framework with two non-equivalent substituents was developed, and constitutional isomers of clathrochelate with two non-equivalent carboxyphenylsulfide groups were synthesized. The interaction of designed iron(II) clathrochelates and their symmetric homologues with globular proteins (serum albumins, lysozyme, β-lactoglobulin (BLG), trypsin, insulin) was studied by protein fluorescence quenching and CD techniques. A highly-intensive ICD output of the clathrochelates was observed upon their association with albumins and BLG. It was shown that in the presence of BLG, different clathrochelate isomers gave spectra of inverted signs, indicating the stabilization of opposite configurations (*Λ* or *Δ*) of the clathrochelate framework in the assembly with this protein. So, we suggest that the isomerism of the terminal carboxy group determined preferable configurations of the clathrochelate framework for the fixation in the protein binding site. MALDI TOF results show the formation of BLG–clathrochelate complex with ratio 1 : 1. Based on the docking simulations, the binding of the clathrochelate molecule (all isomers) to the main BLG binding site (calyx) in its open conformation is suggested. The above results point that the variation of the ribbed substituents at the clathrochelate framework is an effective tool to achieve the specificity of clathrochelate ICD reporting properties to the target protein.