BINDING OF IRON(II) CLATHROCHELATE FUNCTIONALIZED BY SULFOALKYL GROUPS TO ALBUMINS

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Fig.1. The structure (**a**) and CV for 1 mM acetonitrile solutions of disulfoalkyl-terminated iron(II) clathrochelate measured with GC electrode at scan rate 150 mV/s (**b**).

Current task

To examine the interaction of the iron(II) clathrochelate bearing two "flexible" sulfoalkyl-terminated substituents with globular proteins (bovine and human serum albumins (**BSA**, **HSA**), lysozyme (**LYZ**) and beta-lactoglobulin (**BLG**)).

Cyclic voltammograms contain the single quasireversible $Fe^{2+/+}$ reduction wave in the cathodic potential range (-1.2 V) and three irreversible oxidation waves in the anodic potential range, assigned to a metal-centered $Fe^{2+/3+}$ process (0.92 V) and to oxidation of their sulfoalkylsulfide groups (1.05 and 1.16 V).

The redox activity of iron(II) clathrochelate allows potentially to apply it, for example, for sensing of biomolecules

Methods

 Induce circular dichroism (ICD)
Native electrospray ionization mass spectrometry (ESI-MS)

Native Electrospray ionization mass spectrometry



Table 1. Averaged deconvoluted masses of the detected charge states (+15 to +19) of HSA and its adducts with the disulfoalkyl-terminated iron(II) clathrochelate. The mass differences of the observed adducts with respect to nonbound HSA are given.

Species	deconvoluted mass [Da]	mass difference to reference [Da]
Delip. HSA	66'802 ± 21	ref
+ 1 clth	68'140 ± 61	1338
+ 2 clth	68'946 ± 53	2 × 1057
+ 3 clth	69'796 ± 47	3 × 998

Conclusions

The metal complex disulfo-terminated iron(II) clathrochelate with proteins caused an induction of intensive CD outputs in the case of serum albumins and BLG. Molecules of these proteins contain the hydrophobic cavities and nearby positively charged Arg or Lys amino acid residues, which are suggested to promote the formation of the protein–clathrochelate assemblies through electrostatic (polar) interactions.

Native ESI-MS has shown the formation of complexes between disulfoalkyl-terminated iron(II) clathrochelate and HSA with composition 1:1, 1:2 or 1:3 albumin to clathrochelate molecules.

Acknowledgements

The project is funded by the EU Horizon 2020 research and innovation programme under Marie Skłodowska-Curie grant agreement № 778245.

CD spectroscopy



Fig.2. CD-spectra of disulfoalkyl-terminated iron(II) clathrochelate, $Cclth = 20 \mu M$ with different proteins, *mdeg*: BSA (12), HSA (16.4), LYZ (1.3) and BLG (20), *Cproteine* = 40 μ M in 0.05M Tris HCI, pH 7.9.