9th International Conference "Nanotechnologies and Nanomaterials"NANO-2021, 25 - 28 August, Lviv, Ukraine

Supramolecular binding of the designed *meta*- and *para*-carboxyl-terminated monoribbed-difunctionalized Iron(II) clathrochelate isomers to a transport albumin's macromolecule

Chornenka N.V.[1], *Vakarov S.V.*[1], *Kovalska V.B.*[2], *Gumienna-Kontecka E.*[3], *Voloshin Y.*[4]

[1] *V.I. Vernadsky Institute of General and Inorganic Chemistry NASU, Kyiv. e-mail:nina.v.chornenka@gmail.com*

[2] *Institute of Molecular Biology and Genetics, NASU, Kyiv.*

[3] *Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland.*

[4] *A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia.*

Changes in the shapes and in the intensities of the clathrochelate-based induced CD (ICD) spectra of clathrochelate – protein assemblies are known to reflect both the conformation transitions of proteins macromolecules and their structural alterations [1-3].

Current task

To examine the interaction of the *meta*- and *para*-carboxyl-terminated monoribbed-difunctionalized Iron(II) clathrochelate isomers with human serum albumin (HSA) by Induce circular dichroism (ICD) method.

Results

ICD spectrum of the HSA – clathrochelate **2** assembly contains two negative (350 and 520 nm), and one positive (440 nm) bands, ΔICD=11.1 mdeg, while that for its *meta*-substituted analog **1** possesses a "classical" possess two maxima and one minimum, ΔICD=17.4 mdeg (Fig.2).

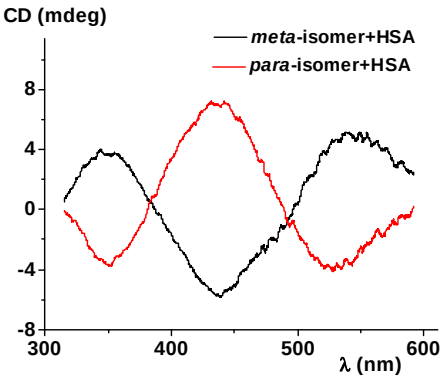

Fig.2. ICD spectra of the HSA – clathrochelate (*meta*- and *para*-isomers) assemblies. These spectra were measured at $c_{protein}$ = 4·10^{-5} and c_{clt} = 2·10^{-5} mol·L^{-1} in 0.05 M tris–HCl aqueous buffer with pH 7.9 at 25°C.

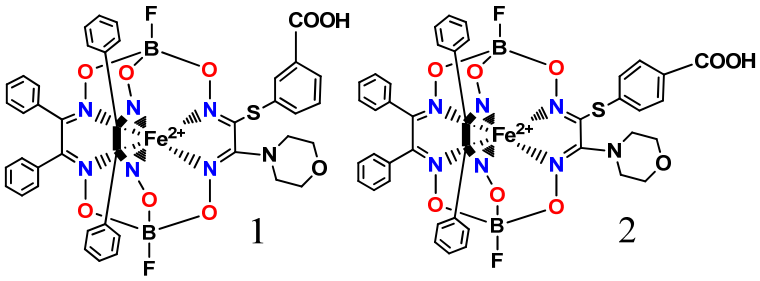

Fig. 1. *meta*- and *para*-carboxyl-terminated constitutional isomers (**1** and **2**) of a monomorpholinemonocarboxyphenylsulfide iron(II) clathrochelate with two functionalizing biorelevant *vic*-substituents [3].

Conclusions

1. Thus, iron(II) clathrochelates **1** and **2** were found to give a pronounced CD output upon their binding to globular protein HSA.
2. The constitutional isomerism of these clathrochelates (*meta*- or *para*-position of the single terminal carboxyl group) is found to strongly affect induced CD-activity of clathrochelates upon their binding to protein, in its presence, possessing the inverted shapes.
3. So, the cage iron(II) complexes of this type are prospective for the design of the proteinsensitive ICD reporters.

References

1. *RSCAdv.,2019,9,24218–24230; doi: 10.1039/c9ra04102h.*
2. *Biomolecules 2020,10, 1602;doi:10.3390/biom10121602.*
3. *Russian Journal of Inorganic Chemistry, 2020, Vol. 65, No. 10, pp. 1513–1521.*

Acknowledgements

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