

## Sensing of a protein's structure using the induced circular dichroism spectra by the monocarboxyphenylsulfide iron(II) clathrochelates as optical reporters.

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Artykuł

### Streszczenie

CD testing of a supramolecular binding of three constitutional isomers (*ortho*-, *meta*-, and *para*-substituted) of an inherently CD-silent monomethinemonocarboxyphenylsulfide iron(II) clathrochelate to globular proteins (serum albumins BSA and HSA, lysozyme and  $\beta$ -lactoglobulin) was performed. This type of isomerism is found to strongly affect an induced CD-activity of these clathrochelates upon their binding to protein. To study an effect of the additional ribbed functionalization on protein's sensing properties, the CD outputs of clathrochelate analogs with biorelevant morpholine group were studied. Such a functionalization is found to substantially affect the protein's CD-sensing properties; this is explained by a formation of hydrogen bonds between this substituent and aminoacid residues of a protein binding site, thus affecting and altering an arrangement of the corresponding clathrochelate-protein assembly. Molecular docking calculations were performed for structural modeling of the BSA-clathrochelate assemblies and to estimate an energy of these supramolecular processes.

### Słowa kluczowe

clathrochelates, iron complexes, globular proteins, albumins, host-guest compounds, induced chirality, optical reporters

### Adres publiczny

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### Strona internetowa wydawcy

<http://link.springer.com>