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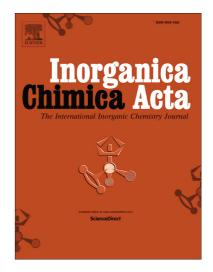
Three Zn(II) complexes with a sexidentate N_2O_4 -donor bis-Schiff base ligand: Synthesis, characterization, DFT studies, in-vitro antimicrobial evaluation and molecular docking studies

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| PII: | \$0020-1693(17)30487-5 |
|------------|---|
| DOI: | http://dx.doi.org/10.1016/j.ica.2017.05.037 |
| Reference: | ICA 17606 |

To appear in: Inorganica Chimica Acta

Received Date:27 March 2017Revised Date:15 May 2017Accepted Date:16 May 2017



Please cite this article as: H. Wang, X. Zhang, Y. Zhao, D. Zhang, F. Jin, Y. Fan, Three Zn(II) complexes with a sexidentate N₂O₄-donor bis-Schiff base ligand: Synthesis, characterization, DFT studies, in-vitro antimicrobial evaluation and molecular docking studies, *Inorganica Chimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.ica. 2017.05.037

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Three Zn(II) complexes with a sexidentate N₂O₄-donor bis-Schiff base ligand:

Synthesis, characterization, DFT studies, in-vitro antimicrobial evaluation and

molecular docking studies

Hu Wang^a, Xia Zhang^a, Yu Zhao^a, Dongmei Zhang^a, Fan Jin^b*, Yuhua Fan^a*

a Key Laboratory of Marine Chemistry Theory and Technology, Ministry of Education, College of Chemistry and Chemical Engineering, Ocean University of China, Qingdao, China

b Max Planck Institute for Terrestrial Microbiology & LOEWE Center for Synthetic Microbiology (SYNMIKRO), Marburg, Germany

Abstract Three Zn(II) complexes with a sexidentate N2O4-donor bis-Schiff base ligand, namely $C_{36}H_{34}N_2O_8 = 1,2$ -bis(2-methoxy-6-formylphenoxy)ethane-L-phenylalanine; L_2 , $C_{28}H_{34}N_2O_8S_2 = 1,2$ -bis(2-methoxy-6-formylphenoxy-6-formylph 1,2-bis(2-methoxy-6-formylphenoxy)ethane-L-methionine; C40H36N4O8 La. = 1,2-bis(2-methoxy-6-formylphenoxy)ethane-L-tryptophan) were synthesized and fully characterized by physico-chemical and spectroscopic methods. The X-ray crystallography shows that the metal atoms of three complexes are all six-coordinate with two nitrogen atoms from C=N groups, two oxygen atoms from ether groups and two carboxylic oxygen atoms in the mono-ligand, forming a distorted octahedral geometry. Theoretical studies of the three complexes were carried out by density functional theory (DFT) Becke's three-parameter hybrid (B3LYP) method employing the 6-31G basis set. Moreover, the antimicrobial activities of the complexes were evaluated against Escherichia coli and Staphylococcus *aureus* by the agar-well diffusion method. The experiment showed that complex 2 exhibited the highest antimicrobial activity. At the same time, molecular docking was investigated to determine the molecular interaction of the complexes with microbial synthase. The docking simulation exhibited that complex 2 was well embedded into the active pocket of the enzyme and showed a more stabilized

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