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Research paper

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**Three Zn(II) complexes with a sexidentate N<sub>2</sub>O<sub>4</sub>-donor bis-Schiff base ligand:  
Synthesis, characterization, DFT studies, in-vitro antimicrobial evaluation and  
molecular docking studies**

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**Abstract** Three Zn(II) complexes with a sexidentate N<sub>2</sub>O<sub>4</sub>-donor bis-Schiff base ligand, namely Zn(C<sub>36</sub>H<sub>34</sub>N<sub>2</sub>O<sub>8</sub>)·2CH<sub>3</sub>OH (**1**), Zn(C<sub>28</sub>H<sub>34</sub>N<sub>2</sub>O<sub>8</sub>S<sub>2</sub>)·CH<sub>3</sub>OH (**2**) and Zn(C<sub>40</sub>H<sub>36</sub>N<sub>4</sub>O<sub>8</sub>)·3CH<sub>3</sub>OH (**3**), (L<sub>1</sub>, C<sub>36</sub>H<sub>34</sub>N<sub>2</sub>O<sub>8</sub> = 1,2-bis(2-methoxy-6-formylphenoxy)ethane-L-phenylalanine; L<sub>2</sub>, C<sub>28</sub>H<sub>34</sub>N<sub>2</sub>O<sub>8</sub>S<sub>2</sub> = 1,2-bis(2-methoxy-6-formylphenoxy)ethane-L-methionine; L<sub>3</sub>, C<sub>40</sub>H<sub>36</sub>N<sub>4</sub>O<sub>8</sub> = 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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