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Metal based pharmacologically active agents: Synthesis, structural characterization, molecular modeling, CT-DNA binding studies and *in vitro* antimicrobial screening of iron(II) bromosalicylidene amino acid chelates



Laila H. Abdel-Rahman^a, Rafat M. El-Khatib^a, Lobna A.E. Nassr^a, Ahmed M. Abu-Dief^{a,*}, Mohamed Ismail^a, Amin Abdou Seleem^b

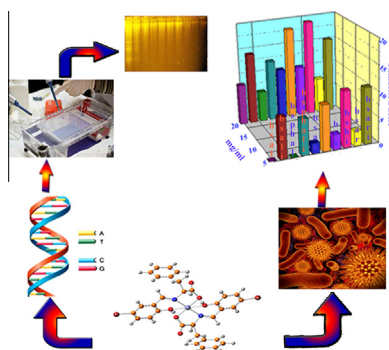
^aChemistry Department, Faculty of Science, Sohag University, 82534 Sohag, Egypt

^bZoology Department, Faculty of Science, Sohag University, 82534 Sohag, Egypt

HIGHLIGHTS

- Novel Schiff base amino acid iron(II) chelates were designed and synthesized.
- They were characterized by different physicochemical and molecular modeling studies.
- DNA binding ability of the investigated complexes was studied using different tools.
- Biological activities have also been performed against different strain of organisms.

GRAPHICAL ABSTRACT



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ABSTRACT

In recent years, great interest has been focused on Fe(II) Schiff base amino acid complexes as cytotoxic and antitumor drugs. Thus a series of new iron(II) complexes based on Schiff bases amino acids ligands have been designed and synthesized from condensation of 5-bromosalicylaldehyde (bs) and α -amino acids (*L*-alanine (ala), *L*-phenylalanine (phala), *L*-aspartic acid (aspa), *L*-histidine (his) and *L*-arginine (arg)). The structure of the investigated iron(II) complexes was elucidated using elemental analyses, infrared, ultraviolet–visible, thermogravimetric analysis, as well as conductivity and magnetic susceptibility measurements. Moreover, the stoichiometry and the stability constants of the prepared complexes have been determined spectrophotometrically. The results suggest that 5-bromosalicylaldehyde amino acid Schiff bases (bs:aa) behave as dibasic tridentate ONO ligands and coordinate to Fe(II) in octahedral geometry according to the general formula $[\text{Fe}(\text{bs:aa})_2] \cdot n\text{H}_2\text{O}$. The conductivity values between 37 and 64 $\text{ohm}^{-1} \text{mol}^{-1} \text{cm}^2$ in ethanol imply the presence of nonelectrolyte species. The structure of the complexes was validated using quantum mechanics calculations based on accurate DFT methods. Geometry optimization of the Fe-Schiff base amino acid complexes showed that all complexes had octahedral coordination. In addition, the interaction of these complexes with (CT-DNA) was investigated at pH = 7.2, by using UV–vis absorption, viscosity and agarose gel electrophoresis measurements. Results indicated that the investigated complexes strongly bind to calf thymus DNA via intercalative mode and showed a different DNA binding according to the sequence: bsari > bshi > bsali > bsasi > bsphali. Moreover, the prepared compounds are screened for their *in vitro* antibacterial and antifungal activity against three types of bacteria, *Escherichia coli*, *Pseudomonas aeruginosa* and *Bacillus cereus* and three types of anti

* Corresponding author. Tel.: +20 1064162700.

E-mail address: ahmed_benzoic@yahoo.com (A.M. Abu-Dief).