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## Synthesis, characterization, X-ray crystal structure, DFT calculation, DNA binding, and antimicrobial assays of two new mixed-ligand copper(II) complexes



S. Yousef Ebrahimipour<sup>a,\*</sup>, Iran Sheikhshoae<sup>a</sup>, Maryam Mohamadi<sup>a,b</sup>, Sebastian Suarez<sup>c</sup>, Ricardo Baggio<sup>d</sup>, Moj Khaleghi<sup>e</sup>, Masoud Torkzadeh-Mahani<sup>f</sup>, Ali Mostafavi<sup>a</sup>

<sup>a</sup> Department of Chemistry, Faculty of Science, Shahid Bahonar University of Kerman, Kerman, Iran

<sup>b</sup> Department of Chemistry, Payame Noor University (PNU), 19395-4697 Tehran, Iran

<sup>c</sup> Departamento de Química Inorgánica, Analítica y Química, Física/INQUIMAE-CONICET, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina

<sup>d</sup> Gerencia de Investigación y Aplicaciones, Centro Atómico Constituyentes, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina

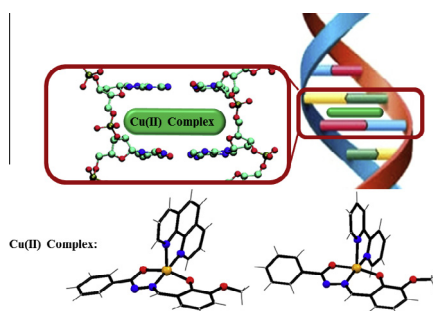
<sup>e</sup> Department of Biology, Faculty of Science, Shahid Bahonar University of Kerman, Kerman, Iran

<sup>f</sup> Department of Biotechnology, Institute of Science, High Technology and Environmental Science, Graduate University of Advance Technology, Kerman, Iran

### HIGHLIGHTS

- A series of ternary mixed ligand Cu(II) complexes were synthesized and characterized.
- The structures of Cu(II) complexes were determined by single crystal X-ray diffraction.
- Investigation of DNA–complex interactions was performed by several experimental methods.
- The antimicrobial activities of the compounds were evaluated against microorganisms.

### GRAPHICAL ABSTRACT



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### ABSTRACT

Two new Cu(II) complexes, [Cu(L)(phen)] (**1**), [Cu(L)(bipy)] (**2**), where L<sup>2-</sup> = (3-methoxy-2-oxidobenzylidene)benzohydrazidato, phen = 1,10 phenanthroline, and bipy = 2,2' bipyridine, were prepared and fully characterized using elemental analyses, FT-IR, molar conductivity, and electronic spectra. The structures of both complexes were also determined by X-ray diffraction. It was found that, both complexes possessed square pyramidal coordination environment in which, Cu(II) ions were coordinated by donor atoms of HL and two nitrogens of heterocyclic bases. Computational studies were performed using DFT calculations at B3LYP/6-311+G(d,p) level of theory. DNA binding activities of these complexes were also investigated using electronic absorption, competitive fluorescence titration and cyclic voltammetry studies. The obtained results indicated that binding of the complexes to DNA was of intercalative mode. Furthermore, antimicrobial activities of these compounds were screened against microorganisms.

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\* Corresponding author at: Department of Chemistry, Faculty of Science, Shahid Bahonar University of Kerman, 76169-14111 Kerman, Iran. Tel./fax: +98 34 3132 2143.

E-mail addresses: [Ebrahimipour@uk.ac.ir](mailto:Ebrahimipour@uk.ac.ir), [Ebrahimipour@ymail.com](mailto:Ebrahimipour@ymail.com) (S.Y. Ebrahimipour).