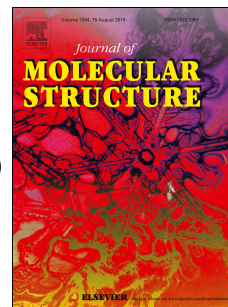


# Accepted Manuscript

Synthesis, characterization, DFT studies of piperazine derivatives and its Ni(II), Cu(II) complexes as antimicrobial agents and glutathione reductase inhibitors

Neslihan Özbek, Serhat Mamaş, Türkan Erdoğan, Saliha Alyar, Kerem Kaya, Nurcan Karacan



PII: S0022-2860(18)30777-4

DOI: [10.1016/j.molstruc.2018.06.076](https://doi.org/10.1016/j.molstruc.2018.06.076)

Reference: MOLSTR 25363

To appear in: *Journal of Molecular Structure*

Received Date: 11 May 2018

Revised Date: 16 June 2018

Accepted Date: 18 June 2018

Please cite this article as: N. Özbek, S. Mamaş, Tü. Erdoğan, S. Alyar, K. Kaya, N. Karacan, Synthesis, characterization, DFT studies of piperazine derivatives and its Ni(II), Cu(II) complexes as antimicrobial agents and glutathione reductase inhibitors, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.06.076.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

**Synthesis, characterization, DFT studies of piperazine derivatives and its Ni(II), Cu(II) complexes as antimicrobial agents and glutathione reductase inhibitors**

**Neslihan Özbek<sup>1\*</sup> Serhat Mamaş<sup>2</sup> Türkan Erdoğan<sup>2</sup> Saliha Alyar<sup>3</sup> Kerem Kaya<sup>4</sup> Nurcan Karacan<sup>2</sup>**

<sup>1</sup>Department of Primary Education, Faculty of Education, Ahi Evran University, Kırşehir, Turkey

\*Corresponding author: E-mail: [nozбек@ahievran.edu.tr](mailto:nozбек@ahievran.edu.tr)

<sup>2</sup>Department of Chemistry, Science Faculty, Gazi University, Ankara, Turkey

<sup>3</sup>Department of Chemistry, Science Faculty, Karatekin University, Çankırı, Turkey

<sup>4</sup>Department of Chemistry, Faculty of Science and Letters, Istanbul Technical University, Istanbul, Turkey

**Abstract**

1,4-Piperazinediacetic acid and 1,4-diethyl ester (**1**) were prepared by treating 1,4-piperazine with ethylchloroacetate; and its structure was identified by single crystal X-ray diffraction analysis. Then, 1,4-piperazinediacetic acid, 1,4-dihydrazide (**2**) and its metal complexes (**2-Ni(II)** and **2-Cu(II)**) were synthesized, respectively. Their structures were characterized by elemental analysis, ESI-MS, IR and NMR spectral data. The electrochemical behavior of compounds was investigated using cyclic voltammetry (CV). The density functional theory (DFT) was used for geometry optimization, HOMO and LUMO energies, HOMO–LUMO energy gap and dipole moment of the compounds. It has been observed that the calculated band gaps for complexes are much smaller than ligands. Furthermore, <sup>13</sup>C and <sup>1</sup>H NMR analyses of (**1**) and (**2**) compounds were performed at B3LYP/6-311++G(d,p) level of theory and compared with the experimental findings. Observed <sup>13</sup>C and <sup>1</sup>H NMR chemical shifts were very good agreement with calculated chemical shifts. The antibacterial activities of synthesized compounds were studied against three Gram-positive and three Gram-negative

Download English Version:

<https://daneshyari.com/en/article/7807005>

Download Persian Version:

<https://daneshyari.com/article/7807005>

[Daneshyari.com](https://daneshyari.com)