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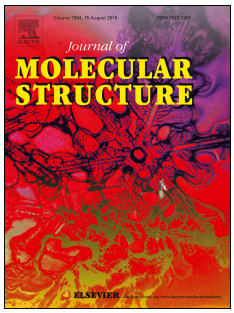

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Synthesis, characterization, DFT studies of piperazine derivatives and its Ni(II), Cu(II) complexes as antimicrobial agents and glutathione reductase inhibitors

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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, ^{13}C and ^{1}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 ^{13}C and ^{1}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