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Synthesis, characterization, DFT studies, molecular docking and *in vitro* anti-bacterial activity of pyrazolone *p*-flurophenylhydrazone and its copper and manganese complexes

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This research focuses on the synthesis, characterization, computational studies and *in vitro* antibacterial studies of pyrazolone phenylhydrazone and its transition metal complexes of copper and manganese. Pyrazolone *p*-Flurophenylhydrazone has been synthesized and characterized using FT-IR, ^{1}H NMR and mass spectrometry. In the same way pyrazolone Cu (II) and Mn (II) transition metal complexes have been synthesized and characterized using FT-IR, ESI mass spectrometry, UV-Visible spectrometry and powder X-ray diffraction (XRD). In addition to these, Quantum mechanical Density Functional Theorycalculations have been simulated for ligand and metal complexes in order to obtain the electronic and structural properties and reactivity of the molecules. Furthermore, molecular docking studies have been carried out on Cu and Mn metal complexes with *E. coli* zinc deformylase inhibitor protein to access the interaction and binding of molecule with respect to the target site of receptor and compared with standard drugs Penicillin-G and Ampicillin. The antibacterial efficiency of ligand and its metal complexes have been evaluated against Gram-Positive and Gram-Negative bacterial assays to investigate its antimicrobial potential. These findings aid in the discovery of new successful leads with potential antimicrobial properties that can be optimized in future to get an effective drug candidates.

Keywords: 4-Acylpyrazolone, *p*-Flurophenylhydrazine, Computational chemistry, Density Functional Theory, Molecular docking, *in vitro* antimicrobial assay