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Transition metal complexes of 2-(2-(1H-benzo[d]imidazol-2-yl)hydrazono)propan-1-ol: Synthesis, Characterization, Crystal structures and anti-tuberculosis assay with docking studies

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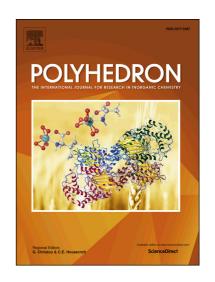
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## **ACCEPTED MANUSCRIPT**

Transition metal complexes of 2-(2-(1H-benzo[d]imidazol-2-yl)hydrazono)propan-1-ol: Synthesis, Characterization, Crystal structures and anti-tuberculosis assay with docking studies

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Abstract: Transition metal coordination complexes of Co(II), Ni(II), Cu(II) and Zn(II) with a newly designed ligand, 2-(2-(1H-benzo[d]imidazol-2-yl)hydrazono)propan-1-ol have been synthesized and characterized using various spectro-analytical techniques. The molecular structures of Co(II), Cu(II) and Zn(II) complexes are determined by single-crystal X-ray diffraction method. The metal to ligand stoichiometry has been found to be 1:2 in the case of Cobalt(II), Nickel(II) and Zinc(II) whereas 1:1 in the case of Copper(II) complex. The newly synthesized ligand and complexes have been assessed for their growth inhibiting potencies against H37Rv strain of *Mycobacterium tuberculosis*. The copper and cobalt complexes have emerged to be potent in vitro growth inhibitors of H37Rv. All the complexes are inhibiting the growth of other tested common microbial flora to a significantly lesser extent, making them selective towards H37Rv in the preliminary analysis. The Consensus scores obtained by the docking studies of the molecules to the target protein enoyl acyl carrier protein reductase of *M. tuberculosis* H37Rv are in good agreement with the obtained MIC values.

**Key Words**: 2-(2-(1H-benzo[d]imidazol-2-yl)hydrazono)propan-1-ol, 2-hydrazinobenzimidazole, transition metal complexes, antituberculosis against H37Rv, enoyl acyl carrier protein reductase of *M. tuberculosis* H37Rv, docking of metal complexes.

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