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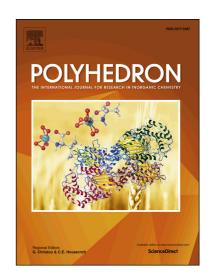
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DNA/BSA interaction, bio-activity, molecular docking simulation study and electrochemical properties of hydrazone Schiff base derived Cu(II)/Ni(II) metal complexes: Influence of the nuclearity and metal ions

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Abstract

Three new transition metal complexes of a tridentate Schiff base ligand, $H_2L = N-(2-1)$ hydroxybenzylideneamino) benzamide, were synthesized in the presence of pyridine, 3methylpyridine and the corresponding metal salts, and were characterized by FT-IR, UV-Vis and Raman spectroscopies, and cyclic voltammetry (CV). The crystal structures of the three complexes, $[Cu^{II}_{2}(L)_{2}(py)_{2}] \cdot 2ClO_{4}(1)$, $Cu^{II}_{2}(L)_{2}(3-Mepy)_{2}(ClO_{4})_{2}(2)$ and $[Ni^{II}(L)(py)_{3}]ClO_{4}$ (3), were determined through X-ray crystallography. In the Cu complexes two different kinds of contacts were be found: shorter (in typical ranges) and longer (Cu-O around 2.5 Å), which assemble the complexes into dimers. The coordination geometry is (taking into account the longer contacts) square-pyramidal in 1, while complexes 2 and 3 show an octahedral geometry. Numerous biological studies have been conducted on H₂L and complexes 1-3. In vitro, their antibacterial activities were examined against Gram-positive and Gram-negative bacteria. The results of these studies indicated that all compounds had antibacterial activity against Gram-positive bacteria. Furthermore, binding studies of H_2L and its complexes with calf thymus DNA (CT-DNA) were studied. Results analyzing the binding of H_2L and the complexes to CT-DNA revealed a hyperchromic effect and a non-intercalative mode of binding. These observations also indicate significant alterations of the bovine serum albumin

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