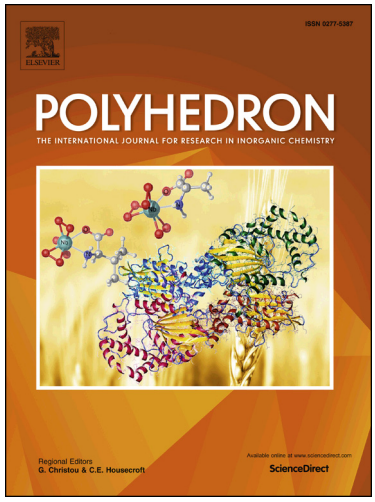

DNA/BSA interaction, bio-activity, molecular docking simulation study and electrochemical properties of hydrazone Schiff base derived Cu(II)/Ni(II) metal complexes: Influence of the nuclearity and metal ions

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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-hydroxybenzylideneamino) benzamide, were synthesized in the presence of pyridine, 3-methylpyridine 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**), $Cu^{II}_2(L)_2(3\text{-Mepy})_2(ClO_4)_2$ (**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 **H_2L** 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