Indian Journal of Chemistry
Vol. 63, October 2024, pp. 1044-1052
DOI: 10.56042/ijc.v63i10.12807

Spectral, anticancer and molecular docking studies of paddle-wheel complex tetrakis(μ-acetato) bis(2-pyridone)dicopper(II) against MCF-7 cell line

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Received 28 July 2024; accepted (revised) 23 September 2024

Tetrakis(μ-acetato)bis(2-pyridone)dicopper(II) (Cu_2TAP) has been obtained unexpectedly during refluxing of HPMP, 2-methyl pyridine and $CuCl_2$ in ethanol in 1:1:1mole ratio. The metal complex has been characterized by FT-IR, Raman, UV-Vis and EPR spectroscopy. The complex shows characteristic NH and CO stretching in IR and Raman. UV-Vis shows bands at 293 and 242 nm due to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions. The compound emits strong fluorescence bands at 726 and 765 nm when excited at 360 and 380 nm respectively. EPR indicates a strong anti-ferro magnetic interaction between the two Cu (II) centers as bridged by the acetate ligands. The cytotoxicity activity has been performed by the MTT assay against MCF-7 breast cancer cells. The binding modes of Cu_2TAPin the active pocket of the target protein Human estrogen receptor alpha (PDB ID: HERT) has been found to be the H-bonding and weak metal-protein interaction. The complex-HERT interaction energy is –8.40 kcal/mol compared to its interaction with doxorubicin (–7.90kcal/mol). Thus Cu_2TAP can be considered as an anticancer agent and may have OLED applications.

Keywords: Tetrakis(u-acetato)bis(2-pyridone)dicopper(II) (Cu_2TAP), Spectral studies, Anticancer activity, Molecular docking