

عنوان مقاله:

Copper Based N,N-Dimethyl-N-(1-Pyridinylmethylidene) Propane-1,3-Diamine Compound: Synthesis, Characterization, and Its Application toward Biocidal Activity

محل انتشار:

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خلاصه مقاله:

The N³ tridentate ligand N,N-dimethyl-N-(1-pyridinylmethylidene) propane-1,3-diamine (DPMPD) and its copper complex (CDPMPD) were synthesized of which metal complex is found in green colour powdered form. The associated spectroscopic techniques were used to characterize both ligand and the metal complex. Powder XRD method was utilized using the Scherrer formula to accomplish the grain size of the metal complex. It was found that the experimental results of the powdered complex were quite similar to that of the reference material with JCPDS ID 00-024-1977. In vitro anticancer activity shows that the metal complex exhibits a moderate cytotoxic effect on Hep-G2 cell line. This cytotoxic phenomenon is well supported by a molecular docking study using target topoisomerase II crystal structure (PDB id 4FM9). The HOMO- LUMO energy gap, predicted from the DFT study, signifies that the complex is susceptible to chemically reactive.

کلمات کلیدی:

DPMPD, CDMPD, anticancer activity, DFT, Docking

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