(البحث رقم 11 في القائمة)

Synthesis, spectroscopic, characterization, X-ray single crystal, DNA			عنوان البحث:
interaction, DFT and molecular docking studies of a new Schiff base ligand			(باللغة الأنجليزية)
derived from 1-((2-hydroxy-2-phenylethylimino)methyl)naphthalen-2-ol,			
and some transition metal; Mn(II), Fe(II), Co(II), Ni(II), Cu(II), and Pd			
(II) complexes			
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Shehata ,Matti Haukka , Rania G. Mohamed			المؤلفون: (باللغة الأنجليزية)
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ملخص موجز للبحث:

The emergence and rapid spread of cancer cells has highlighted the urgent need for advanced anti-cancer therapies. The widespread use of transition metal complexes as metalloids prompted us to synthesize and characterize novel coordination complexes of Mn(II), Fe(II), Co(II), Ni(II), Cu(II), and Pd(II) using spectroscopic analysis, with a novel Schiff base ligand (H2L). This novel base was obtained from the condensation of 2amino-1-phenylethan-1-ol and 2-hydroxy naphthaldehyde. Conventional single-crystal X-ray diffraction (SCXD) successfully revealed the structure of the H2L ligand. X-ray diffraction data revealed that the ligand existed as a zwitterion, an ion possessing both positive and negative electrical charges. Thermal analysis demonstrated the high stability of the complexes. The antimicrobial activity of some of the complexes was studied. The DNA binding activity was also investigated using optical spectroscopy and gel electrophoresis. Furthermore, molecular modeling of the complexes and ligands was examined. A molecular docking study of the complexes was also performed. According to the results, the copper complex bound to DNA more strongly than the other complexes under study. Therefore, the copper complex can be used as an important source of potent .biological activity