

Synthesis, characterization and biological studies of S-4-methylbenzyl- β -N-(2-furylmethylene)dithiocarbazate (S4MFuH) its Zn²⁺, Cu²⁺, Cd²⁺ and Ni²⁺ complexes

ABSTRACT

S-4-methylbenzyl- β -N-(2-furylmethylene)dithiocarbazate (S4MFuH, 1) derived from the condensation reaction of furaldehyde (Fu) with S-4-methylbenzylidithiocarbazate (S4MBDTC) has been complexed with transition metal acetates to give Zn(S4MFu)₂ (2), Cd(S4MFu)₂ (3), Cu(S4MFu)₂ (4) and Ni(S4MFu)₂ (5). It is evident from the shift in $\nu(\text{CN})$ and $\nu(\text{NN})$ in the IR spectra of the complexes that deprotonated 1 acts as a bidentate ligand coordinating through the azomethine nitrogen and thiolato sulfur atoms. This was confirmed by single crystal X-ray diffractometry. The U-shaped dithiocarbazate 1 exists in the E configuration with the thione bond anti to the azo bond. A change in conformation is noted in the transition metal complexes resulting from deprotonation and NS-chelation. 2 and 3 display a distorted tetrahedral geometry with the major cause of the distortion being two close intramolecular M...O interactions. Binding interaction studies with calf thymus DNA demonstrated that 4 also had the strongest DNA binding affinity ($K_b=2.85 \times 10^4 \text{M}^{-1}$) among all compounds prepared in this work. The Cu(II) complex, 4, was also moderately active against estrogen receptor-positive breast cancer cells, MCF-7 ($\text{IC}_{50}=3.02 \mu\text{M}$) while the remainder were inactive against MCF-7 and all showed no activity towards receptor negative breast cancer cells, MDA-MB-231.

Keyword: S-4-methylbenzylidithiocarbazate; Furaldehyde; Transition metal complexes; NS bidentate Schiff base; Single crystal X-ray diffraction; Cytotoxic activity