

## New insight into the structural, electrochemical and biological aspects of macrocyclic Cu(II) complexes derived from S-substituted dithiocarbazate Schiff bases

### ABSTRACT

Copper (II) complexes synthesized from the products of condensation of S-methyl- and S-benzylthiocarbazate with 2,5-hexanedione (SMHDH2 and SBHDH2 respectively) have been characterized using various physicochemical (elemental analysis, molar conductivity, magnetic susceptibility) and spectroscopic (infrared, electronic) methods. The structures of SMHDH2, its copper (II) complex, CuSMHD, and the related CuSBHD complex as well as a pyrrole byproduct, SBPY, have been determined by single crystal X-ray diffraction. In order to provide more insight into the behaviour of the complexes in solution, electron paramagnetic resonance (EPR) and electrochemical experiments were performed. Antibacterial activity and cytotoxicity were evaluated. The compounds, dissolved in 0.5% and 5% DMSO, showed a wide range of antibacterial activity against 10 strains of Gram-positive and Gram-negative bacteria. Investigations of the effects of efflux pumps and membrane penetration on antibacterial activity are reported herein. Antiproliferation activity was observed to be enhanced by complexation with copper. Preliminary screening showed Cu complexes are strongly active against human breast adenocarcinoma cancer cell lines MDA-MB-231 and MCF-7.

**Keyword:** Dithiocarbazate; Schiff base; Macroacyclic ligand; Tetradentate ligand; NNSS ligand; Copper complexes; Bioactivity; MDA-MB-231; MCF-7; Gram-positive; Gram-negative