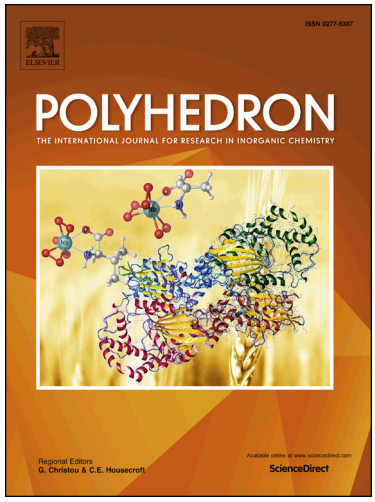

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Copper(II)-Sulfonamide Schiff base complexes : Structure, biological activity and theoretical interpretation

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$[(SMX\text{-}N{=}C\text{-}C_6H_2(o,p\text{-}Cl_2)\text{-}O)]_2Cu$ (**1**) and $[(STZ\text{-}N{=}C\text{-}C_6H_2(o,p\text{-}Cl_2)\text{-}O)]_2Cu$ (**2**) (SMX : Sulfamethoxazole; STZ : Sulfathiazole) have been characterized by spectroscopic data and the structural confirmation of **2** has been carried out by single crystal X-ray diffraction studies. The structure shows distorted square pyramid geometry and ligand serves as N, O chelator and OH_2 occupies the axial position. Packing shows hydrogen bonded 1D chain and π---π interaction generates 2D supramolecular structure. Anticancer activity of the complexes against human breast cancer cell (MDA-MB 231) lines shows considerably low IC_{50}, 82 μM (**1**) and 53 μM (**2**). DNA interaction of the complexes, **1** and **2**, determines the binding constants 1.515 x 10^5 M^{-1} (**1**) and 1.164 x 10^5 M^{-1} (**2**). Docking studies have been performed with the DNA structure (PDB id 1ZEW) to establish drug activity by groove binding.

Keywords: Sulfonamide Schiff bases, Cu(II) complex, X-ray structure, anticancer activity, DFT computation.