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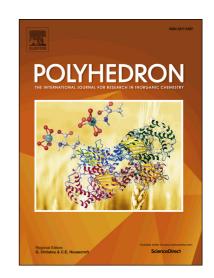
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Copper(II)-Sulfonamide Schiff base complexes: Structure, biological activity and theoretical interpretation

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[(SMX-N=C-C₆H₂(o,p-Cl₂)-O)]₂Cu (1) and [(STZ-N=C-C₆H₂(o,p-Cl₂)-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 OH₂ 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 IC₅₀, 82 μ M (1) and 53 μ M (2). DNA interaction of the complexes, 1 and 2, determines the binding constants 1.515 x 10⁵ M⁻¹ (1) and 1.164 x 10⁵ 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.

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