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

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$[(\text{SMX}-\text{N}=\text{C}-\text{C}_6\text{H}_2(o,p\text{-Cl}_2)\text{-O})]_2\text{Cu}$  (**1**) and  $[(\text{STZ}-\text{N}=\text{C}-\text{C}_6\text{H}_2(o,p\text{-Cl}_2)\text{-O})]_2\text{Cu}$  (**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 pyramidal geometry and ligand serves as N, O chelator and OH<sub>2</sub> occupies the axial position. Packing shows hydrogen bonded 1D chain and  $\pi\cdots\pi$  interaction generates 2D supramolecular structure. Anticancer activity of the complexes against human breast cancer cell (MDA-MB 231) lines shows considerably low IC<sub>50</sub>, 82  $\mu\text{M}$  (**1**) and 53  $\mu\text{M}$  (**2**). DNA interaction of the complexes, **1** and **2**, determines the binding constants  $1.515 \times 10^5 \text{ M}^{-1}$  (**1**) and  $1.164 \times 10^5 \text{ M}^{-1}$  (**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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