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Green Synthesis, Molecular Docking, Antimicrobial and antioxidant activity of Schiff base ligands

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Abstract

Schiff base ligand of ofloxacinthrough the condensation of 2- aminothiazolehave been synthesizedwith the help of microwave irradiation.. These ligands were characterized by IR and NMR techniquesand investigated for in vitro antibacterial and antioxidant activity. Ligand has shown remarkable antibacterial activity (Minimum inhibitory concentration 8-16 lg/ml) comparable to commercial antibiotic Ciprofloxacin. To check out the binding mode Molecular studies were carried out. Anticancer activity of synthesized compounds against Squamous Cell Carcinoma (SCC4), head and neck cancer cell line has also been studied at different concentrations and at different time points. Ligands have shown remarkable anticancer results (IC50 31.1 and 43.1 lM) against the tested cell line in concentration dependent manner. Molecular docking studies were carried out to find the binding mode of the synthesized macrocyclic Schiff base ligand to Epidermal Growth Factor Receptor (EGFR) Kinase (PDB ID: 1M17).

Keywords: Ofloxacin, 2-aminothiazole, antibacterial, antioxidant and Molecular Docking