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Synthesis, Characterisation, biological activity and Docking studies of ternary metal complexes of Cu(II) and Co(II with 4-chloro-2-(2-Hydroxy) Naphthylidene Amino Benzothiazole Schiff base and Glycine ligands

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Abstract

The ternary complexes of Cu(II), Co(II) containing 4-chloro-(2-hydroxy)Naphthylidene aminobenzothiazole Schiff base and Glycine ligandwere synthesised. These compounds were characterised by elemental analysis, FT-IR, UV-Vis, mass, TGA, molarconductance and SEM. From the electronic spectra and magnetic moment values the geometry of the complexes was determined. TGA data confirmed that there are no coordinated water molecules in the complexes. The binding mode of the Schiff base ligand to metal ions through azomethine nitrogen, oxygen of aldehyde and N, O donors of the glycine ligand was confirmed through the absorption bands appeared in the IR spectrum. Anticancer activity of the compounds revealed that Schiff base ligand and its Cu(II), Co(II) complexes have shown greater activity against the HeLa and MCF-7 cell lines. The complete cleavage of CT-DNA occured with the Cu(II), Co(II) ternary complexes. The In vitro antimicrobial assessment of the Schiff base and its complexes have displayed that complexes have shown more activity than its free ligand. Docking studies were carried out on ligand to illustrate binding mode of ligand in to different active sites which are Pencillin binding protein 4 of Staphylococcus aureus , Penicillin Binding Protein 4 (dacB) of E.coli and Homo sapiens cyclin dependent kinase.

Keywords: Ternary metal complexes, IR, SEM, Antibacterial, DNA cleavage anticancer activity.

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