A New Carbazole Substituted Thiosemicarbazon Cu(II) Complexes: Spectroscopic, Molecular Docking and Cytotoxic Studies

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N-ethyl substituted 9-ethylcarbazolethiosemicarbazone (ECCAET) and its copper(II) complex [Cu(ECCAET)$_2$] were synthesized, and characterized by analytical and spectroscopic techniques. Interaction of the ligand and complex with CT-DNA and BSA was investigated using molecular docking studies. Cytotoxicity of compounds was also evaluated against human lung cancer (A549), human colorectal cancer (HT29), and non-cancerous L929 fibroblast cell line as a control cell line. Molecular docking studies showed that copper(II) complexes of thiosemicarbazone molecule strongly interacted with CT-DNA and BSA. Furtherly, Cu(ECCAET)$_2$ was highly toxic when compared to ECCAET, according to the IC_{50} values. Cu(ECCAET)$_2$ was also more effective against A549 and HT29 cancer cells. It can be deduced that Cu(ECCAET)$_2$ will contribute to the development of new potential anticancer agents and to the understanding of the mechanism of biomolecules.

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