Synthesis, Structural Elucidation, Cytotoxic, Density Functional Theory and Molecular Docking Studies of Anti-Inflammatory Drugs Cu(II) Complexes

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Abstract:

New metal(II) complexes were synthesized by reacting copper(II) chloride dihydrate (Cu(II) in the form of $MCl_2{\cdot}2H_2O$) with the drugs Pitavastatin and Rosuvastatin. The characterization of these metal complexes was carried out using various spectroscopic techniques, including elemental analysis, molar conductance measurements, magnetic moment analysis, FT-IR spectroscopy, and EPR spectroscopy. Additionally, thermogravimetric analysis (TGA) and kinetic studies were performed. The IR spectra suggested that the ligands coordinated in a bidentate binding mode, utilizing the oxygen atoms of the carboxylate group in both ligands. Molar conductivity measurements indicated that all the complexes were non-electrolytic in nature. Additionally, results from magnetic moment analysis and EPR spectroscopy revealed that the complexes exhibited octahedral geometries. Thermal studies were conducted to confirm the structures and assess the thermal stability of the complexes. The thermodynamic parameters were determined using the Coats–Redfern and Horowitz–Metzger methods. Additionally, a DNA binding study was performed through spectrophotometric experiments and viscosity measurements, which revealed that the complexes act as groove binders to DNA. The synthesized complexes exhibited significant cytotoxic activity, demonstrating strong inhibition against both breast carcinoma (MCF-7) and human lung cancer cell lines. Furthermore, the results from molecular docking revealed a strong correlation with the experimental findings related to cytotoxicity. These results suggest that the synthesized complexes have the potential to be effective anticancer agents.

Keywords:

Metal-based complex, Statin drugs, DNA binding, Anticancer properties, Molecular docking.