In silico and *in vitro* studies of transition metal complexes derived from curcumin–isoniazid Schiff base

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Abstract

A series of transition metal complexes have been synthesized from biologically active curcumin and isoniazid Schiff base. They are characterized by various spectral techniques like UV-Vis, Fourier transform infrared (FT-IR), nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) and mass spectroscopies. Moreover, elemental analysis, magnetic susceptibility and molar conductivity measurements are also carried out. All these data evidence that the metal complexes acquire square planar except zinc(II) which adopts a tetrahedral geometry, and they are non-electrolytic in nature. Groove mode of binding between the calf thymus DNA (CT DNA) and metal complexes is confirmed by electronic absorption titration, viscosity and cyclic voltammetry studies. In addition to that, all the metal complexes are able to cleave pUC 19 DNA. Optimized geometry and ground-state electronic structure calculations of all the synthesized compounds are established out by density functional theory (DFT) using B3LYP method which theoretically reveals that copper(II) complex explores higher stability and higher biological accessibility. This is experimentally corroborated by antimicrobial studies. *In silico* Absorption, Distribution, Metabolism, Excretion (ADME) studies reveal the biological potential of all synthesized complexes, and also biological activity of the ligand is predicted by PASS online biological activity prediction software. Molecular docking studies are also carried out to confirm the groove mode of binding and receptor-complex interactions.

Keywords: DFT calculation; Isoniazid; antimicrobial; groove binding; in silico ADME; molecular docking.