Synthesis, characterization, ADMET, *in vitro* and *in vivo* studies of mixed ligand metal complexes from a curcumin Schiff base and lawsone

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Abstract

Complexes are currently synthesized from plant origin because of their therapeutic effect against certain diseases with toxicity. Hence, in this work, four new transition metal(II) mixed ligand complexes have been synthesized using a curcumin Schiff base (primary ligand) and lawsone (as co-ligand). The geometry of these complexes was explored by elemental analyses, molar conductance, thermal analysis, magnetic moment values, IR, NMR, Mass, electronic and EPR spectral studies. Electronic absorption titrations, viscosity measurements and molecular docking studies reveal that all the metal complexes interact with the CT DNA by groove binding. Among all the complexes, the copper(II) complex (complex 1) exhibits a higher K_b value (3.5×10^{-4} M) which reveals that it has a strong binding efficiency toward the CT DNA. The complexes also possess strong DNA cleavage efficiency. Cytotoxicity investigations on *Artemia salina* show that all the complexes possess higher cytotoxic effect than the ligand. Moreover, all the metal complexes have better antimicrobial efficacy than the ligand. Swiss ADME, PASS and pkCSM online softwares are helpful to predict the pharmacokinetic and biological actions of the curcumin Schiff base. Theoretical results obtained from the *in silico* study are experimentally corroborated by *in vivo* anti-inflammatory screening study. All the above studies demonstrate that the copper complex possesses biological activity similar to that of the drug like molecules.