In silico and biological exploration of greenly synthesized curcumin-incorporated isoniazid Schiff base and its ruthenium complexes

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Abstract

In the present investigation, ultrasound-mediated three Knoevenagel condensates have been prepared from biologically active curcumin and different aldehydes. Curcumin Schiff bases have been prepared by reacting these Knoevenagel condensates with isoniazid. Ruthenium Schiff base complexes are synthesized and octahedral geometry of these complexes are confirmed by various analytical techniques like elemental analysis, molar conductive measurements, and spectroscopic techniques like UV–Vis, FT-IR, NMR, EPR, and ESI mass. Moreover, optimized geometry and DFT calculation have been done using Gaussian 09 W software and the quantum mechanical calculation of these complexes is also performed. Pharmacokinetic behavior of the synthesized compounds is examined using SWISS ADME, PASS online, and molinspiration online software. Based on this, in vivo and in vitro pharmaceutical investigations are carried out and it is found that all the complexes possess potent biological activity than the ligand. All the synthesized compounds are docked against 1BNA and 4fm9 colon cancer receptors. Interestingly, intercalative binding efficacy of the synthesized compounds is confirmed by using UV–visible absorption titration and viscosity measurements against CT-DNA.