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Synthesis, structural, pharmacological and molecular docking simulations studies of some transition metal complexes(Article)

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Abstract

Neutral [CuL_2], [NiL_2], [CoL_2], [MnL_2] and [ZnL_2] complexes were synthesized using Schiff base derived from Benzalidene-4-imino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one and tyrosine. All the compounds were characterized by elemental analysis, magnetic susceptibility, ESI-Mass spectra, Powder XRD, SEM, FTIR, UV–Vis., ^{1}H & ^{13}C NMR, EPR and Cyclic voltammogram techniques. The general formula of the complexes [ML_2] was confirmed by analytical data and ESI-mass spectra. The polycrystalline nature of the complexes was proved by powder XRD and surface morphology studies ensure that the complexes exist in nano size grain. The octahedral geometry of synthesized complexes was examined by magnetic susceptibility measurements and electronic absorption spectra. ESR parameters of copper complex clearly indicate that the complex is axially elongated octahedral geometry. Pharmacological activities like analgesic, antipyretic, anti-inflammatory and CNS activities of Schiff base and its metal complexes were studied using albino mice which show that chelates have higher activities than free ligand. The good antioxidant activity of chelates was observed through DPPH free radical scavenging assay method. The antimicrobial activities of Schiff base and its complexes reveal that the complexes have superior antimicrobial activity than Schiff base. The DNA binding interaction study of [CuL_2] by UV–Vis. spectroscopy shows the strong binding of [CuL_2] complex on DNA with high binding constant value ($K_b = 7.4 \times 10^5$) and the respective binding occurs through intercalation mode. The prediction of activity spectra of substance (PASS) expounds the drug-like nature of the compound. The in silico ADMET studies expose that Schiff base acquires enhanced biological potential. This was further confirmed by molecular docking studies of complex with DNA and (PDB ID: 6COX) protein. © 2020 Elsevier B.V.

Author keywords

Anti-inflammatory | Antimicrobial activity | Antioxidant assay | Antipyretic activity | ESR spectra | Molecular docking simulations studies | Schiff base | Transition metal chelates

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