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Applied Organometallic Chemistry

Volume 36, Issue 6, June 2022, Article number e6704

Synthesis, spectroscopic, in vitro, in silico, and in vivo studies of binuclear Cu (II), Ni (II), Ru (II), and Zn (II) complexes with tetradentate Schiff base ligand(Article)

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Abstract

A novel Schiff base macrocyclic ligand was synthesized by the condensation of 4-(3,4-diaminophenyl)benzene-1,2-diamine with β-naphthol-1-aldehyde. Binuclear complexes were synthesized from this Schiff base by reaction with Cu (II), Ni (II), Ru (II), and Zn (II) metal salts. Square planar geometrical structures of Cu (II), Ni (II), and Ru (II) complexes were achieved by several physicochemical methods, namely UV–Vis, FT-IR, NMR, ESI-Mass, and thermogravimetric analysis, respectively. Density functional theory (DFT) calculations at the B3LYP/6-31G(d) level were carried out to gain an insight into the thermodynamic stability and biological accessibility of the complexes. Moreover, molecular docking analysis was done against a novel target protein PDB: 6M71 (SARS-CoV-2). Both the Schiff base ligand and metal complexes showed excellent interaction with protein receptor. All the metal complexes have the strong tendency to undergo intercalation mode of binding with CT DNA. All the in vivo and in vitro screening studies showed that the complexes exhibit higher activities than the free Schiff base. © 2022 John Wiley & Sons Ltd.

Author keywords

binuclear | DFT | in vitro | in vivo | molecular docking

Indexed keywords

Engineering controlled terms: Chelation | Complexation | Copper compounds | Density functional theory | Ligands | Molecular modeling | Nickel compounds | Proteins | Ruthenium compounds | SARS | Synthesis (chemical) | Thermogravimetric analysis | Zinc compounds

Engineering uncontrolled terms: Binuclear | Density-functional-theory | In-silico | In-vitro | In-vivo | Molecular docking | Schiff-base | Schiff-base ligands | Synthesised | Vivo studies

Engineering main heading: Metal complexes

Funding details

Funding text

We express our sincere thanks to the Head, Principal, and The Madura College Managing Board for providing the research facilities and their constant encouragement. We thank Prof. Dr. P. Natarajan, Department of Pharmaceutical chemistry, Sankaralingam Bhuvaneswari College of Pharmacy, Annaikuttam, Sivakasi, for in vivo and in vitro studies.