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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](#)

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[Metal complexes](#)

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