# Insight into the *in vitro* anticancer screening, molecular docking and biological efficiency of pyridine-based transition metal(II) complexes

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## Abstract

The undesirable effects caused by the chemotherapeutic drugs are already in use, mainly the platinated compounds requiring amendments for which many potential scaffolds resembling the activity of cisplatin are explored. Herein, the DNA binding, cleavage, molecular docking, antimicrobial proficiency, and cytotoxic nature of four non-platinated transition metal(II) complexes incorporating pyridine moiety were investigated. The complexes adopted octahedral geometry, and the mode of interaction with DNA was explored by absorption spectroscopy, fluorescence spectroscopy, electrochemical technique, and viscosity measurements. These studies indicate a groove-binding mode of the complexes to CT DNA. The stability of the synthesized complexes was investigated at physiological pH. All the complexes exhibited single-strand scission of the supercoiled pBR322 DNA where copper(II) complex (**1**) showed double-strand DNA prominently by converting the supercoiled DNA to linear form. The antimicrobial screening of the complexes yielded expected results. The complexes selectively showed activity against cancer cell lines and less toxicity toward the noncancerous NHDF cell line. Overall, **1** showed superior activity in the biological investigation. These studies reveal that the coordination of transition metal(II) ion with the ligand plays a pivotal role in the enhancement of the biological potential of the complexes.