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Comparison of the *in silico* antibacterial effects of coumarin-based Schiff bases and metal complexes on the DNA gyrase enzyme

Işık Çakmak[a] & Nurhan Gümrükçüoğlu*[b]

[a] Biostatistics and Medical Informatics, Karadeniz Technical University, Trabzon, Türkiye

[b] Department of Medical Services and Techniques, Vocational School of Health Sciences, Karadeniz Technical University, Trabzon, Türkiye

E-mail: ngumrukcuoglu@ktu.edu.tr

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The global increase in antibiotic resistance is reducing the effectiveness of current treatment options and necessitating the development of new antimicrobial agents. Schiff base derivatives and metal complexes are one of the pharmacophore groups that attract attention due to their broad biological effect spectrum and high chemical stability. Metals are important components of many biochemical reactions occurring in living organisms and are among the fundamental cellular elements selected to perform various biological processes in nature. *In silico* approaches offer a significant advantage in the drug discovery process by enabling the examination of candidate molecules at low cost and in a short time. In this study, the potential inhibitory effects of the Cu (II), Zn(II), Ni(II), and Fe (II) metal complexes of the newly designed coumarin derivatives on the *Escherichia coli* DNA gyrase (PDB ID: 1KZN) enzyme were compared using molecular docking methods. The findings revealed that Schiff base metal complexes generally exhibit higher affinity than free ligands. The strongest binding was observed in the Zn-L1 (-10.6 kcal/mol) and Fe-L1/Ni-L2 (-10.3 kcal/mol) complexes. The findings suggest that Schiff base-metal complexes may be evaluated as potential antimicrobial candidates through DNA gyrase inhibition. *In vitro* studies will provide experimental evidence to support the pharmacological potential of these complexes.

Keywords: Schiff base metal complexes, DNA gyrase inhibition, Molecular docking, Antimicrobial resistance