In silico evaluation of usnic acid derivatives to discover potential antibacterial drugs against DNA gyrase B and DNA topoisomerase IV

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ABSTRACT

Due to the rising increase in infectious diseases brought on by bacteria and anti-bacterial drug resistance, antibacterial therapy has become difficult. The majority of first-line antibiotics are no longer effective against numerous germs, posing a new hazard to global human health in the 21st century. Through the drug-likeness screening, 184 usnic acid derivatives were selected from an *in-house* database of 340 usnic acid compounds. The pharmacokinetics (ADMET) prediction produced fifteen hit compounds, of which the lead molecule was subsequently obtained through a molecular docking investigation. The lead compounds, labelled compound-277 and compound-276, respectively, with the substantial binding affinity towards the enzymes were obtained through further docking simulation on the DNA gyrase and DNA topoisomerase proteins. Additionally, molecular dynamic (MD) simulation was performed for 300 ns on the lead compounds in order to confirm the stability of the docked complexes and the binding pose discovered during docking tests. Due to their intriguing pharmacological characteristics, these substances may be promising therapeutic candidate for anti-bacterial medication.

KEYWORDS

Anti-bacterial; docking; MD simulation; usnic acid

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