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Abstract

In Silico Investigation of 2-Aryloxy-1,4-Naphthoquinone Derivatives as Potential Antibacterials Against Escherichia coli

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Abstract: In this research, a comprehensive analysis was conducted on 30 derivatives of naphthoquinone using computational methods such as 3D-QSAR modeling, assessment of drug similarity, ADMET analysis, molecular docking, and molecular dynamics simulations. The primary aim was to establish robust 3D-QSAR models employing CoMFA, aiming to identify potential novel antibacterial agents targeting Escherichia coli. The QSAR models exhibited strong predictive capabilities, as demonstrated by their assessments (Q2 = 0.613, R2 = 0.902, SEE = 0.063). Utilizing the QSAR model predictions, we devised four novel molecular structures. These structures were subsequently evaluated for drug likeness and ADMET predictions, with two compounds displaying exceptional ADMET predictions and drug likeness. Molecular docking was utilized to explore the interactions between the recently designed molecules, denoted as molecules 1 and 2, and the intended protein target. Of these, compound 2 displayed considerable stability based on the results obtained. To validate this stability, extensive molecular dynamics simulations were performed for 100 nanoseconds at three distinct temperatures, affirming the observed high stability.

Keywords: E. coli; QSAR; ADMET; Drug-likness; Molecular dynamics

Supplementary Materials:

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