Molecular docking and *in silico* evaluation of phytochemicals of bioactive methanolic extract of *Ipomoea mauritiana* Jacq. as anti-bacterial agents

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ABSTRACT

Antibacterial treatment has grown difficult due to the increasing growth in bacterial infections, as well as their tolerance to most first-line antibiotics. This is a severe danger to the world's human health in the 21st century, necessitating further research to identify drugs with improved antibacterial effects and broad-spectrum functions. This study aimed to discover anti-bacterial agents through the molecular docking and *in silico* approach. Most responsive thirty (32) compounds on UPLC-Q-TOF/MS analysis were selected from our previous report to get the hit compound(s) against inhibition of cell wall synthesis, inhibition of protein synthesis, interference with nucleic acid synthesis, inhibition of a metabolic pathway, inhibition of membrane function and inhibition of adenosine triphosphate (ATP) synthase. From the molecular docking results, we afforded six compounds for cell wall synthesis protein, four compounds for protein synthesis protein, five for nucleic acid synthesis protein, three for metabolic pathway protein, four for membrane function protein and three for ATP synthase protein which eventually undergoes the pharmacokinetic and drug-likeness properties to obtain lead compound(s). Finally, we discovered that compounds **Turpinionosides B**, **Polydatin**, **Ledebouriellol**, and **Pterodontoside A** have the strongest binding interactions with cell wall synthesis, inhibition of protein synthesis and inhibition of metabolic pathway synthesis, interference with nucleic acid synthesis and inhibition of ATP synthase, inhibition of membrane function proteins, respectively. These compounds have the potential to become an anti-bacterial therapeutic candidate due to their promising pharmacological properties.

KEYWORDS

ADMET and drug-likeness; anti-bacterial; in silico; Ipomoea mauritiana; molecular docking

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