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In vitro and *in silico* study of phytoconstituents from *Hyptis suaveolens* L. for antibacterial potential

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The discovery of new antibacterial molecules is crucial given the increasing resistance of bacteria to existing antibiotics. Therefore, there is a need for new, safer antibacterial therapeutics. Even though *H. suaveolens* has a long history of medicinal use, many of its bioactive compounds remain unidentified. Thus, this study aimed to find novel phytochemicals from the methanolic extract of *H. suaveolens* that may be useful against pathogens. *In vitro* antibacterial testing revealed that the 24th fraction showed significant antibacterial activity, and GC-MS analysis identified several phytochemicals. ADMET analysis showed that 1,2-dihydro-2-oxo-4-quinolyl-2-pyridyl ketone, diethyl phthalate, n-hexadecenoic acid, squalene, and α-tocopherol acetate have drug-like characteristics. Molecular docking of these five ligands was performed against two target proteins using PyRx AutoDock Vina. The targets included intercellular adhesion protein R from *Staphylococcus aureus* and DNA polymerase III subunit beta from *Escherichia coli*. 1,2-dihydro-2-oxo-4-quinolyl-2-pyridyl ketone and diethyl phthalate had the strongest binding affinities and the lowest binding energies. ADMET analysis confirmed that they are drug-like, non-toxic, and non-carcinogenic. These findings suggest that 1,2-dihydro-2-oxo-4-quinolyl-2-pyridyl ketone and diethyl phthalate could be useful antibacterial agents for treating infections.

Keywords: Pathogen, GC-MS analysis, ADMET analysis, molecular docking