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Analysis of molecular docking with essential oil piper cubeba with tuberculosis

Tuberculosis, caused by Mycobacterium tuberculosis, is one of the world's most lethal infectious diseases. Natural compounds are currently the target of pharmacological interest since they have pharmacological properties. Piper cubeba is a type of natural product which already has antibacterial properties. Through these data on Piper cubeba, to theoretically prove its effectiveness against mycobacterium tuberculosis, this study performed a virtual screening of part of its compounds through molecular docking of the 3pty protein with the following ligands a-humulene; b-caryophyllene oxide; b-elemene; eugenol; methyleugenol. The protein was protonated through the Charmm-GUI platform, after that we treated the ligands by the open babel GUI program, and the docking is done through the autodock vina software. Through the affinity energy results when compared with the results of the original ligand AFO1 (-5.6 kcal/mol) it can be concluded that of the targets studied at least two have the potential to be candidates for possible tuberculosis drugs, these being a-humulene (-6.0 kcal/mol) and b-caryophyllene (-6.4 kcal/mol). According to the affinity energies eugenol possessed the same energy as the original ligand and the others did not obtain good energies. The parameter established to determine whether there was a good affinity energy or not, is for the ligand to have energy above the energy of the original ligand (AFO1).

Keywords: Molecular docking; tuberculosis; essential oil; medicinal chemistry; piper cubeba