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Study of the physicochemical properties of compound presents in essential oil of Piper cubeba

Tuberculosis is one of the main causes of infectious deaths in the world, this infection affects about 25% of the world population, caused by Mycobacterium tuberculosis. Statistical data indicate that tuberculosis reached about 10.4 million people in 2016 according to the WHO, in addition to this 80% of deaths in HIV-positive people is due to tuberculosis. Piper cubeba belongs to the Piperaceae family, of oriental origin, widely used as a spice and folk medicine acting in various treatments. For pharmacology, the analysis process via docking is a facilitating tool, enabling the replacement of the random screening method with a virtual computational screening, saving unnecessary expenses and researcher time, analyzing binding energies and drug location deviation with the target protein, however, the molecular modeling process becomes viable for the discovery of new drugs due to the practicality in data processing and the wide possibility of several tests with different molecules. The analysis via docking was performed using the protonated protein obtained through the CHARMM-GUI, the docking process was performed via Auto Dock Vina and, data processing and image acquisition of the interactions was performed using Discovery Studio Visualize. The analyzed ligands presented the following binding energies in kilocalorie per mol: 1,8-cineole (-5.4), α-Terpineol (-5.8), α-Terpinolene (-5.0), β-Acement (-4.6) Terpinen- 4-ol (-5.3). After processing and analyzing data, it is concluded that the selected ligands still had weaker interactions than the original ligand AFO1 (-6.1) present in the protein

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