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Study of the physicochemical properties of Alpha-selinen, Beta-caryophyllene, Myrcene, p-cymene-8-ol, viridiflorol

Tuberculosis affects a large part of the world population, especially in developing countries. The antibiotics isoniazid and ethambutol have been used for decades as first-line drugs for treatment. Mycobacterium tuberculosis infections, the causative agent of, but the rise of multidrug-resistant and extensively drug-resistant strains pose a serious threat to current treatment options. Therefore, the current investigation involved the representation of the structure of the Mycobacterium tuberculosis EmbC (code 3pty) protein with the respective ligands, Alpha-selinen, Beta-caryophyllene, Myrcene, p-cymene-8-ol, viridiflorol. The proposed modified structures of the ligand were designed on a computer. The protein was obtained through the dattabankingrcsb.org platform and protonated through the Charmm-GUI, the ligands were obtained were removed from databanking zinc.docking.org and were treated by the open babel Gui software, and the docking is done through the autodok vina software. Through the results of affinity energy when compared with the result of the original ligand AFO1 (-5.6 kcal/mol) it was concluded that of the studied targets, at least two have potential to be candidates for possible drugs for tuberculosis, being they the alpha selinene (-6.3 kcal/mol) and viridiflorol (-6.2 kcal/mol).

Keywords: Mycobacterium tuberculosis EmbC, Tuberculosis, physicochemical properties.