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Analysis of Cannabinol and Cannabidiol affinity with GBRA1

Authors : Hamid Hossein Khezri, Afsaneh Javdani-Mallak

Abstract : Fast inhibitory neurotransmission in the mammalian nervous system is largely mediated by GABAA receptors, chloride-selective members of the superfamily of pentameric Cys-loop receptors. Cannabidiol (CBD) is one of the members of cannabinoid compounds found in cannabis. CBD and Cannabinol (CBN), as the other extract of plant Cannabis were able to reduce myofascial pain in rats with immunosuppressive and anti-inflammatory activities. In this study, we accomplished protein-protein BLAST, and the sequence was found to be for Gamma-aminobutyric acid receptor subunit alpha-1 (GBRA1) chain A and its 3D structure was subsequently downloaded from Protein Data Bank. The structures of the ligands, cannabinol, and cannabidiol, were obtained from PubChem. After the necessary process of the obtained files, AutoDock Vina was used to perform molecular docking. Docking between the ligands and GBRA1 chain A revealed that cannabinol has a higher affinity to GBRA1 (binding energy = -7.5 kcal/mol) compared to cannabidiol (binding energy = -6.5 kcal/mol). Furthermore, cannabinol seems to be able to interact with 10 residues of the protein, out of which 3 are in the neurotransmitter-gated ion-channel transmembrane domain of GBRA1, whereas cannabidiol interacts with two other residues. Although the results of this project do not indicate the activating /or inhibitory capability of the studied compounds, it suggests that cannabinol can act as a relatively strong ligand for GBRA1.

Keywords : protein-ligand docking, cannabinol, cannabidiol, GBRA1
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