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Abstract

Molecular docking study of *Papaver* alkaloids to some alkaloid receptors

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Background and objectives: More than 40 different alkaloids have been obtained from opium the most important of which are morphine, codeine, papaverine, noscapine and tabaine. Opioid alkaloids produce analgesia by affecting areas of the brain that have peptides with pharmacological pseudo-opioid properties. These alkaloids show important effects on some intracellular peptides like mu, delta, and kappa receptors. Therefore, studying the effects of these alkaloids on different receptors is essential. **Methods:** Molecular docking is a well-known method in exploring the protein-ligand interactions. In this research, five important alkaloids were docked to crystal structure of human mu opioid receptor (4DKL), human delta opioid receptor (4EJ4) and human kappa opioid receptor (4DJH) which were retrieved from protein databank. The 3D-structures of alkaloids were drawn by chembiooffice2010 and minimized with hyperchem package and submitted to molecular docking utilizing autodock-vina. Flexibility of the proteins was considered. The docking studies were performed to compare the affinity of these five alkaloids to the mentioned receptors. **Results:** We computationally docked each alkaloid compound onto each receptor structure and estimated their binding affinity based on dock scores. Dock score is a criteria including binding energy which utilized here for prediction and comparison of the binding affinities. Binding interactions of the docked alkaloids in receptor pockets were also visually inspected and compared. **Conclusion**: In this approach, using docking study as a computational method provided a valuable insight of opioid receptor pocket structures which would be essential to design more efficient drugs in pain managements and addiction treatments.

Keywords: alkaloids, chemometrics, Molecular docking, *papaver* genus

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