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## Basic pharmacophore mapping of a set of plant derived anti-inflammatory compounds through Autodock Vina

Shilpa Chatterjee and Souvik Basak Dr. B.C. Roy College of Pharmacy and Allied Health Sciences, India

Plant based research have led to isolation of myriads of compounds which are reported to have anti-inflammatory activity. But approaches are lacking to design a basic pharmacophore harbouring the potential of inflammation-antagonistic action, together with encompassing the possibility of finding a lead for synthesizing anti-inflammatory class of compounds. As a control study in this aspect, we have chosen a set of such plant borne compounds with anti-inflammatory activity and subjected them to virtual screening by receptor-ligand interaction. The receptor-ligand binding studies have been performed by Autodock Vina where the dock scores have been generated as compounds' binding affinities towards the receptor. Two direct inflammatory pathway enzymes cyclooxygenase- 1 (COX-1) and cyclooxygenase-2 (COX-2) have been chosen as potential receptors and subjected to docking via whole receptor-ligand fitting model. Each compound generated nine possible conformers for receptor fitting with binding affinities as dock scores. The conformation revealing highest binding affinity was adopted as the best active conformation of the associated compound. Thus, a best active conformer based library has been constructed encompassing all the plant derived compounds; from which five superior structures have been used as templates to map the core pharmacophore. To validate the pharmacophore-receptor interaction, amino acid mapping in the ligand binding domain has also been performed. Furthermore, to analyze the receptor-ligand complex, studies involving RMSD calculation to their original lead as well as different bonding interactions have also been undertaken.