

عنوان مقاله:

(Molecular docking and ADME studies of natural compounds against bitter taste receptors(TAS₂Rs

محل انتشار:

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خلاصه مقاله:

A subfamily of 25 G protein-coupled receptors called the human bitter taste receptors (TAS₂Rs) mediates the perception of the bitter taste. The three TAS₂Rs (TAS₂R14, TAS₂R39, and TAS₂R46) stand out from the rest of the TAS₂Rs. Since they are the most widely tuned bitterness receptors, recognize a wide range of chemical, natural, and miscellaneous agonists and antagonists in the micromolar range with extremely low potency. In addition, the receptors are expressed in oral, and several extra-oral tissues, and they are suggested for having salient physiological roles associated with innate immune responses, cancer, and male fertility. In the present study, computational techniques (molecular docking, in silico ADMET, and prediction of drug-likeness) were used to perform virtual screening on 452 natural ligands selected from the bitterDB database. Studies on receptor-ligand binding were carried out by Schrodinger drug discovery Suite. Subsequently, the Glide docking program and extra precision (XP) were applied. The best ligands based on docking score are myricetin (-11.50 Kcal/mol), dihydrofisetin (-9.33 Kcal/mol), and artesin (-9.19 Kcal/mol) for TAS₂R14, TAS₂R39, and TAS₂R46 receptors, respectively. The docking results depict the promising potent natural product which can interact with the TAS₂Rs receptor for therapeutic approaches. Furthermore, higher potency ligands are needed to investigate the mentioned three receptors function and to modulate them for future clinical applications, such as cancer treatment or taste prediction.

کلمات کلیدی:

Bitter Taste Receptor, Molecular Docking, Natural Compound

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