عنوان مقاله:

Synthesis and docking analysis of new heterocyclic system of tetrazolo[۵',۱':۲,۳][۱,۳,۴]thiadiazepino [۷,۶-b]quinolines as aldose reductase inhibitors

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خلاصه مقاله:

Objective(s):In recent years, the chemistry of Tetrazolo[۵',۱':۲,۳][۱,۳,۴]thiadiazepino [۷,۶-b]quinolines have received considerable attention owing to their synthetic and effective biological importance which exhibits a wide variety of biological activity. As the inhibitor of aldose reductase, the aforementioned compounds may have implication in preventing complications of diabetes. Materials and Methods: A group of tetrazolo[۵',۱':۲,۳][۱,۳,۴]thiadiazepino [۷,۶-b]quinolinederivatives were synthesized, and theoretically evaluated for their inhibitory potency against aldose reductase (ALR) via docking process. The docking calculation was done in Genetic Optimization for Ligand Docking (GOLD) ۵.۲ software using Genetic algorithm. Results: Compounds ۳a and ۳f showed the best inhibitory potency by GOLD score value of ۷۸.۸۳ and ۷۶.۸۸ respectively. Conclusion: All of the best models formed strong hydrogen bonds with Trp ۱۱۱ and Tyr ۲۰۹ via tetrazole moiety. It was found that pi-pi interaction between Tyr ۲۰۹, Trp ۲۰ and His ۱۱۰ side chain and quinolin moiety was one of the common factors in enzyme-inhibitor junction. It was found that both hydrogen bonding and hydrophobic interactions are important in the structure and function of biological molecules, .especially for inhibition in a complex

کلمات کلیدی:

Aldose Reductase Inhibitors, Diabetes Mellitus, Docking Analysis, Heterocyclic compound, Quinoline derivatives