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Article Detail

Insilico approaches to demonstrate uzarigenin and calotropagenin as potential carbonic anhydrase II (CAII) inhibitors

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Abstract: Background: Inhibition studies on carbonic anhydrase II (CAII) (EC 4.2.1.1) activity are gaining attention due to their immense therapeutic application in the treatment of cancer, and obesity. Clinically used CAII inhibitors (CAIs), such as acetazolamide, and brinzolamide produce undesirable side effects like depression, and nausea. So non-toxic and natural CAI are being researched with special interest. Steroids such as bile acids, steroidal sulfamates, and sex hormones have previously been shown to significantly inhibit CAII activity. In the current insilico study, cardiotonic steroids (uzarigenin and calotropagenin) have been investigated as possible CAII inhibitors. Objective: To evaluate uzarigenin and calotropagenin as potential inhibitors of carbonic anhydrase II (CAII) activity, using insilico methods Methods and materials: Reverse pharmacophore screening and inverse docking of ligands was performed to identify potential targets. The results were validated by docking study. The binding affinity and interactions of docked ligands viz, uzarigenin, calotropagenin, acetazolamide (standard) and cholic acid (positive control) with CAII macromolecule, was comparatively analyzed. MMPBSA calculation of protein ligand complex were computed to determine the strength of binding.

ADMET analysis was conducted to ascertain drug like properties of ligands. Results and conclusion: Uzarigenin (Ki= -7.6 kcal/mol) and calotropagenin (Ki= -7.9 kcal/mol), by virtue of their interaction with catalytically important residues (Phe130, Ile91, Gln92), good fit score (2.82, and 2.93 respectively), and significant binding energy (? Ebind=-21.18 and -23.57kJ/mol respectively) in MMPBSA calculation can be further investigated as lead CAII inhibitors.

Keyword: Carbonic anhydrase II, cardenolides, reverse pharmacophore, uzarigenin, calotropogenin

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