

Theoretical studies on the anti-inflammatory activity of hyperoside with the lipoxygenase 5 enzyme

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5-Lipoxygenase (LOX-5) is a key enzyme involved in the synthesis of pro-inflammatory leukotrienes and has become an important target for the development of new drugs in the pharmaceutical and biotechnology industries. LOX-5 catalyzes two steps in the biosynthesis of leukotrienes, which are lipid mediators of inflammation derived from arachidonic acid. Leukotriene antagonists are used in the treatment of asthma and have recently gained interest due to their potential role in atherosclerosis therapy.

So, the aim of our study was to perform molecular docking of hyperoside with the LOX-5 enzyme. A molecular docking study was conducted using the tool known as AutoDockTools 1.5.6. Genetic algorithm parameters were applied for ligand interaction, with 10 runs of this criterion. LOX-5 (PDB ID: 2q7m) structure was obtained from PDB database. The resolution of 2q7m was 4.25 Å. The ligand structures of hyperoside (CID_5281643) was obtained from PubChem database. The active site of the docking protein was identified utilizing the Computed Atlas for Surface Topography of Proteins. As a standard was taken diclofenac sodium. We applied the following classification of selectivity: inhibition concentration (IC)₅₀ < 0.001 mM (high selective); 0.05 > IC₅₀ > 0.01 (medium selective); IC₅₀ > 0.05 mM (low selective). The hyperoside had a high value of free energy value (-11.12 kcal/mol), whereas IC₅₀ was 0.00000707 mmol, so hyperoside belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperoside was 45% more than of diclofenac sodium (-6.00 kcal/mol, IC₅₀ – 0.039882 mmol).

It was established that hyperoside is a potentially high selective inhibitor of LOX-5 enzyme. So, the extract with hyperoside can be applied for developing a new anti-inflammatory drugs.