Theoretical studies on the anti-inflammatory activity of hyperoside with the phospholipase A2 enzyme

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Phospholipase A2 catalyzes the hydrolysis of the sn-2 position of membrane glycerophospholipids to liberate arachidonic acid, a precursor of eicosanoids including prostaglandins and leukotrienes. These products are precursors of bioactive eicosanoids and platelet-activating factor which have been implicated in pathological states of numerous acute and chronic disorders.

So, the aim of our study was to perform molecular docking of hyperoside with the phospholipase A2 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. Phospholipase A2 (PDB ID: 3hsw) structure was obtained from PDB database. The resolution of 3hsw was 3.00 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: IC50<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 (-14.05 kcal/mol), whereas IC50 was 0.00000005045 mmol, so hyperecin belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperoside was 50% more than of diclofenac sodium (-7.65 kcal/mol, IC50 – 0.00248 mmol).

It was established that hyperoside is a potentially high selective inhibitor of phospholipase A2 enzyme. So, the extract with hyperecin can be applied for developing a new anti-inflammatory drugs.