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

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The use of anti-inflammatory drugs is often associated with numerous side effects. For example, steroidal medications can lead to osteoporosis, adrenal atrophy, and immune system suppression, while non-steroidal drugs may cause bronchospasms. Given these concerns, the search for new anti-inflammatory compounds derived from herbal sources remains highly relevant. One promising target for such research is the phospholipase A2 enzyme, which plays a crucial role at the beginning of inflammation.

So, the aim of our study was to perform molecular docking of hyperecin 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 hyperecin (CID_3663) 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 hyperecin had a high value of free energy value (-15.34 kcal/mol), whereas IC50 was 0.00000000564 mmol, so hyperecin belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperecin was 50% mo.re than of diclofenac sodium (-7.65 kcal/mol, IC50 – 0.00248 mmol).

It was established that hyperecin 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.