Theoretical studies on the anti-inflammatory activity of hyperecin with the nuclear factor - kB enzyme

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The nuclear factor κB (NF-κB) pathway has long been considered a prototypical proinflammatory signaling pathway, largely based on the role of NF-κB in the expression of proinflammatory genes including cytokines, chemokines, and adhesion molecules. NF-κB has long been considered a prototypical proinflammatory signaling pathway, largely based on the activation of NF-κB by proinflammatory cytokines such as interleukin 1 (IL-1) and tumor necrosis factor α (TNF- α). NF-κB has important roles in the pathogenesis of chronic inflammatory diseases such as rheumatoid arthrtitis.

So, the aim of our study was to perform molecular docking of hyperecin with the NF-KB protein. 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. NF-KB (PDB ID: 1svc) structure was obtained from PDB database. The resolution of 1svc was 3.0 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: inhibition concentration (IC)50<0.001 mM (high selective); 0.05>IC50>0.01 (medium selective); IC50>0.05 mM (low selective).

The hyperecin had a medium value of free energy value (-7.24 kcal/mol), whereas IC50 was 0.00497 mmol, so hyperecin belong to medium selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperecin was 46% more than of diclofenac sodium (-3.90 kcal/mol, IC50 – 1.38 mmol). It was established that hyperecin is a potentially medium selective inhibitor of NF-KB protein. So, the extract with hyperecin can be applied for developing a new anti-inflammatory drugs with treatment chronic diseases.