Theoretical studies on the antioxidant activity of hyperecin with the xanthine oxidase enzyme

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Xanthine oxidase (XOD) are single-gene products that exist in separate but interconvertible forms. XOD utilizes hypoxanthine or xanthine as a substrate and O2 as a cofactor to produce superoxide and uric acid. XOD is reported to play an important role in cellular oxidative status, detoxification of aldehydes, oxidative injury in ischemia-reperfusion, and neutrophil mediation. XOD may serve as a messenger or mediator in the activation of neutrophil, T cell, cytokines, or transcription in defense mechanisms rather than as a free radical generator of tissue damage.

The aim of our study was to perform molecular docking of hyperecin with the xanthine oxidase 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. XOD (PDB ID: 1fiq) structure was obtained from PDB database. The resolution of 1svc was 2.5 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 high value of free energy value (-9.41 kcal/mol), whereas IC50 was 0.00012756 mmol, so hyperecin belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperecin was 49% more than of diclofenac sodium (-4.17 kcal/mol, IC50 – 0.88 mmol).

It was established that hyperecin is a potentially medium selective inhibitor of xanthine oxidase. So, the extract with hyperecin can be applied for developing a new antioxidant drugs for preventing oxidative stress.