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

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Xanthine oxidase (XOD) is an enzyme that exists in different but interconvertible forms, encoded by a single gene. It catalyzes the oxidation of hypoxanthine and xanthine, using oxygen as a cofactor, to generate uric acid and superoxide. XOD is recognized for its significant role in regulating cellular redox balance, aldehyde detoxification, oxidative damage during ischemia-reperfusion, and neutrophil activation. Rather than solely acting as a source of free radicals that cause tissue damage, XOD may function as a signaling molecule or mediator in immune responses, influencing neutrophil activation. The aim of our study was to perform molecular docking of hyperoside 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 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 (-8.61 kcal/mol), whereas IC50 was 0.00048606 mmol, so hyperoside belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperoside was 46% more than of diclofenac sodium (-4.17 kcal/mol, IC50 – 0.88 mmol).

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