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

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NADPH oxidase is an enzyme responsible for the intentional generation of reactive oxygen species (ROS) and plays a key role in regulating redox-dependent processes in various biological systems. It is found both in phagocytic and nonphagocytic cells. This enzyme facilitates the transfer of electrons from intracellular NADPH across the membrane, combining them with molecular oxygen to form superoxide anion, a highly reactive free radical. As a result, NADPH oxidase is a critical contributor to oxidative stress development. The aim of our study was to perform molecular docking of hyperoside with the NADPH 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. NADPH oxidase (PDB ID: 5oOx) structure was obtained from PDB database. The resolution of 1svc was 3.0 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 (-9.81 kcal/mol), whereas IC50 was 0.00006497mmol, so hyperoside belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperoside was 51% more than of diclofenac sodium (-4.76 kcal/mol, IC50 – 0.3245 mmol).

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