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

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The NADPH oxidase catalyze the deliberate production of reactive oxygen species (ROS) and are established regulators of redox-dependent processes across diverse biological settings. NADPH oxidases are present in phagocytes and in a wide variety of nonphagocytic cells. The enzyme generates superoxide by transferring electrons from NADPH inside the cell across the membrane and coupling them to molecular oxygen to produce superoxide anion, a reactive free-radical. So, NADPH oxidase is a crucial enzyme in developing oxidative stress.

The aim of our study was to perform molecular docking of hyperecin 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 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 (-11.64 kcal/mol), whereas IC50 was 0.00000208 mmol, so hyperecin belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperecin was 59% more than of diclofenac sodium (-4.76 kcal/mol, IC50 – 0.3245 mmol).

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

Theoretical studies on the antioxidant activity of hyperecin with the myeloperoxidase enzyme

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Myeloperoxidase (MPO) is a member of the superfamily of heme peroxidases that is mainly expressed in neutrophils and monocytes. MPO-derived reactive species play a key role in neutrophil antimicrobial activity against various pathogens. However, activation of MPO can catalyze the reaction of chloride and H_2O_2 to produce HOCl. MPO also mediates oxidative stress by promoting the production of reactive oxygen species (ROS), modulating the polarization and inflammation-related signaling pathways. MPO can be a therapeutic target for attenuating oxidative damage in ischemic stroke. The aim of our study was to perform molecular docking of hyperecin with the myeloperoxidase 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. MPO (PDB ID: 3f9p) 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).