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

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Myeloperoxidase (MPO) is an enzyme from the heme peroxidase superfamily, primarily found in neutrophils and monocytes. MPO-generated reactive species are essential for neutrophil defense mechanisms against pathogens. However, MPO activation facilitates the reaction between chloride and hydrogen peroxide (H_2O_2), leading to the formation of hypochlorous acid (HOCl). Additionally, MPO contributes to oxidative stress by enhancing reactive oxygen species (ROS) production and influencing polarization as well as inflammation-related signaling pathways. The objective of our study was to conduct molecular docking of hyperoside 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 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 (-8.06 kcal/mol), whereas IC50 was 0.00123 mmol, so hyperoside belong to high selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperoside was 51% more than of diclofenac sodium (-4.65 kcal/mol, IC50 – 0.39 mmol).

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