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).

The hyperecin had a high value of free energy value (-9.19 kcal/mol), whereas IC50 was 0.00018505 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 (-4.65 kcal/mol, IC50 – 0.39 mmol).

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

Relation structure and action of antimicrobial activity α-arbutin, β-arbutin and hydroquinone

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Arbutin (C12H16O7) is aglucopyranoside of hydroquinone with two different configurations: alpha (α) and beta (β). The β-isomer can only be obtained from medicinal raw materials, and inturn, the α-isomer is its synthetic analog; the main difference between these isomers is that instead of β-glucose there is α-glucose. Hydroquinone is an aromatic compound which consists of benzyl and 2 OH groups in para-positions. Hydroquinone is a highly toxic compound and is carcinogenic.

All over the world, arbutin-containing medicinal raw materials (lingonberry and bearberry leaves) are used for the treatment and prevention of cystitis, glomerulonephritis and pyelonephritis, as uroseptic, diuretic and antiazotemic agents

According to this theory, arbutin has a uroseptic effect only due to the action of hydroquinone and nothing more, it turns out that arbutin does not have an antimicrobial effect at all, which is also a contradiction. In our opinion, the discussion