Theoretical studies on the anti-inflammatory activity of hyperoside with the nuclear factor - KB enzyme

[1]Maslov O. Yu., [2]Komisarenko M. A., [1]Kolisnyk S. V., [1]Bondarenko N. Yu.

[1]Department of General Chemistry,

[2]Department of Pharmacognosy and Nutriciology,

National University of Pharmacy, Kharkiv, Ukraine

alexmaslov392@gmail.com

The NF-κB pathway is widely recognized as a key proinflammatory signaling mechanism due to its role in regulating the expression of proinflammatory genes, including cytokines, chemokines, and adhesion molecules. Its activation is triggered by proinflammatory cytokines such as interleukin-1 (IL-1) and tumor necrosis factor-alpha (TNF-α). NF-κB plays a crucial role in the development of chronic inflammatory diseases, including rheumatoid arthritis.

So, the aim of our study was to perform molecular docking of hyperoside with the NF-KB protein.

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. NF-KB (PDB ID: 1svc) 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 low value of free energy value (-4.24 kcal/mol), whereas IC50 was 0.78 mmol, so hyperoside belong to medium selective inhibitor. Comparing result with diclofenac sodium standard, the affinity of hyperoside was 8% more than of diclofenac sodium (-3.90 kcal/mol, IC50 – 1.38 mmol).

It was established that hyperoside is a potentially low selective inhibitor of NF-KB protein.