18th National and 3rd International Conference of Iranian Biophysical chemistry
هجدهمین همایش ملی و سومین همایش بین المللی بیوشیمی فیزیک ایران
25-26 Des, 2024, University of Hormozgan
۶-۵ دی ماه ۱۴۰۳، دانشگاه هرمزگان

Investigation of chrysin as interleukin 6 potential inhibitor by *in silico* method

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Abstract

Rheumatoid arthritis (RA) is a chronic inflammatory autoimmune disease distinguished by painful inflammation of the joints (1). Cytokines such as IL-6 have a crucial role in the initiation and development of rheumatoid inflammation. IL (interleukin)-6 is a multifunctional cytokine essential for hematopoiesis, immunology, bone metabolism, and inflammation (2, 3). This study aimed to investigate the molecular mechanism of chrysin in the treatment of rheumatoid arthritis (RA) using molecular docking approach. Molecular docking studies were performed using Autodock software. The 3D structure of the chrysin was obtained from Pubchem and converted into PDB format by AutoDock software for docking analysis. Afterward, the IL6 protein was taken from the Protein Data Bank (PDB), molecular docking was done with chrysin by using the Autodock software. Then, the obtained results were analyzed by Chimera software. Molecular docking shown high binding affinity for the chrysin to IL6 protein. The ligands interacted with IL6 residues in the active site of the protein, which may be important for IL6 inhibitory activity. This study can provided evidence to consider the chrysin as natural product with further research in vitro and in vivo in the treatment of the rheumatoid arthritis.

Key words: Rheumatoid arthritis, Chrysin, Molecular docking

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