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Faculty of Basic Sciences

Department of Chemistry

The Thesis Submitted for the Degree of M.Sc (in the field of Bioinformatics)

Bioinformatic evaluation of the inhibitory effect of a number of bile acids derivatives on the activity of Leptospira interrogans bacteria

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Abstract:

Bile acids form a large family of molecules that consist of a steroid structure with four rings, a side chain of five or eight carbons that ends in a carboxylic acid, and several hydroxyl groups. Their number and orientation are different among certain groups. Leptospira are long and slender bacteria. There are two types of Leptospira introgans and Leptospira biflexa, the first of which contains human pathogenic bacteria and causes an infectious disease called leptospirosis. Bile acid derivatives have an inhibitory effect on the activity of Leptospira interrogans bacteria. Leptospirosis manifests itself in different clinical forms, such as acute, subacute, and chronic, as well as a form without clinical symptoms. In this research, the inhibitory effect of a number of bile acid derivatives on the activity of Leptospira interrogans bacteria is investigated using molecular docking, and the binding method of triterpenoid derivatives to the active site of the target protein will be evaluated. The presence of hydrophilic and hydrophobic groups in these derivatives enables them to create different interactions with the active site of the target protein. The X-ray crystal structure of the target protein of Leptospira interrogans is taken from the protein database: (PDB: lpxc) In the ligand preparation stage, the structures of the studied ligands, bile acid derivatives, will be optimized using the Gaussian 09 software package under the **B3LYP/6-31g basis set. Auto Dock Vina and MOE software will be used to add compounds to the protein receptor. Among all the investigated derivatives of bile acids, the derivative that has the lowest energy among the others is more suitable, considering that it is more stable than the other derivatives. According to the investigations, the best composition is the derivative of 10 bisyl acid, followed by the derivative of 13 bisyl acid.

Key words: bile acid, docking, Leptospira interrogans, ursolic acid, molecular attachment, HIV-1 protease enzyme, inhibitor