



University of Zabol

Graduate school

Faculty of Basic Sciences

Department of Chemistry, Department of Organic Chemistry

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

**Investigation of molecular docking of a number of triterpenoid  
derivatives on *Leptospira interrogans* bacteria**

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## **Abstract :**

Triterpenoids with the molecular formula  $C_{30}H_{48}$  contain 6 isoprene units and are derived from the 30-carbon acyclic compound squalene. Most of the terpenoids are tetracyclic and pentacyclic. Alcohols, aldehydes, ketones or carboxylic acids may be found in terpenoids. In this research, the antibacterial and antimicrobial effect of a number of triterpenoid derivatives on *Leptospira interrogans* bacteria will be investigated using molecular docking, the way of binding triterpenoid derivatives to the active site of LpxC protein. The crystal structure of the target protein of *Leptospira interrogans* is taken from the protein database.

In the stage of ligand preparation, the structure of the studied ligands of triterpenoid derivatives will be optimized using Gossin software under the \*\*B3LYP/6-31g basis set. MOE software is used to dock the compounds into the protein receptor. will take Then, using MOE software, ligand and solvent molecules were removed from the bacterial code and saved in MOE format, then using MOE software, docking of bacteria with crystal structure was done.

The results show that the interactions of these derivatives with the triterpenoid enzyme play an important role. In inhibiting this enzyme, in addition, some derivatives formed hydrogen bonds and van der Waals interactions with this enzyme.

**Key words:** triterpenoid, *Leptocypera*, molecular docking, protein, enzyme, inhibition