



University of zabol  
Graduate school  
Faculty of science  
Department of chemistry

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

**Title:**

**Theoretical study of inhibitory ability of some  
acridine derivatives against cholinesterase enzymes  
for treatment of Alzheimer's disease**

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**Abstract**

Tacrine is one of the first known inhibitors of cholinesterase enzymes. This drug including three rings that central ring is *para*-substituted pyridine one. It seems that changing electronic properties of side ring lead to change of overall electronic properties and influences on inhibitory strength of it. Also, it is expected that this method can optimize some of properties of drug and control side effects of it. In this research, initial structures of some acridines are optimized using quantum mechanical computations and then molecular docking studies are performed for investigating role of different substituents on inhibitory strength of them against cholinesterase enzymes. In addition, effects of different factors such as charge transfer, electron charge densities, nucleophilicity, electrophilicity, and etc. on inhibitory strength of them are evaluated.

**Keywords:** Acridine, Molecular docking, Cholinesterase, Inhibitor