Abstract

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Department of: Pharmaceutical chemistry and drug control

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Title of Thesis: **Molecular modeling study of potential acetylcholinesterase inhibitors.**

This diploma thesis deals with an utilization of molecular docking to confirm the ability to inhibit acetylcholinesterase and butyrylcholinesterase in several substances. Well known AChE inhibitors (donepezil, tacrine, galanthamine, huperzine A) were chosen as ligands binding to active site of the enzyme. Their activity was confirmed. Other substances with certain inhibition potential were studied and in most cases the potential was proven. Structures of cholinesterases from human body and *Torpedo californica* were used for studies. The experimental part was carried out on a computer using a molecular modeling software: MGL Tools, PyMOL, Chimera and Autodock Vina.