Abstract

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Title of Diploma Thesis: **Molecular modeling study of potential mycobacterial enoyl ACP reductase inhibitors.**

Tuberculosis is a worldwide spread infectious disease. The biggest problem of our time are completely and multi resistant strains of *Mycobacterium tuberculosis* that do not respond to currently known drugs. The main reason for high resistance and drug resistance is a bacillus composition of its cell wall. It contains a high proportion of mycolic acids. The synthesis of mycolic acids takes several steps. The final step is a catalytic reduction by enzyme enoyl - ACP reductase (InhA).

This work was focused on finding new potential substances that would be able to inhibit this enzyme. There were used methods of computing and molecular modeling to search these substances. Adjusting of crystallographic structures ran in the program Maestro and docking in the MOE program. Over the 30 000 thousand molecules from the ZND (Zinc Natural Derivates) were tested by molecular docking on 3 crystallographic structures of InhA enzyme. 8 of these molecules were selected from this amount because their docking results suggest that these molecules have potential inhibitory effect.