Section 2
Summary of the Project

Malaria, the most severe infectious disease, afflicts nearly 500 million people and kills about 2 million annually. *Plasmodium falciparum* and *Plasmodium vivax*, the two malaria species responsible for the most infections and deaths, are becoming increasing resistant to drugs, making it essential to identify new antimalarail agents. Proteases are attractive candidates for drug development because they play vital roles in parasite metabolism. Hemoglobin degradation is a metabolic process that is central to the growth and maturation of the malaria parasite. Two aspartic proteases from *Plasmodium falciparum* that initiate degradation, plasmepsin (Plm) I and II, have been identified and characterized. In this project the hemoglobin degradation enzyme Plm II is used as the target macromolecule. Computer assisted database search method was used to dock molecules into the active site of Plm II using the computer software Dock version 4. Docked compounds were ranked according to their interaction energy score with the active site and the binding energy of some selected compounds were calculated using the computer software MOLARIS. In order to check the selectivity of the selected compounds they were docked into a similar enzyme, cathepsin D found in humans and their binding energies were also calculated. Based on binding energy values ten compounds were identified as potential antimalarial drug leads.