Antimalaria In Silico Screening against the Target of Plasmodium falciparum Enoyl Acyl Carrier Protein Reductase (PFENR) using Indonesia Natural Compound Database (Poster Presentation) - International Seminar on Medicinal Chemistry and Timmerman Award Surabaya, October 15, 2011

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ABSTRACT

Malaria is one of problematic infectious diseases worldwide. The absence of an effective vaccine and the spread of drug resistant strains of Plasmodium clearly indicate the necessity for the deveplopment of new chemotherapeutic agents. Recent method being developed is searching a new drug of antimalarial using in silica screening, or also know as virtual screening. One of enzyme target that important for growth of the malaria parasite is P/asmodium /a/ciparum Enoyl' Acyl Canier Protein Reductase (PfENR). Inhibition of this enzyme cause the fatty acid biosynthesis type ll will be tem1inated. In this research, in silica screening was performed using GOLD softwa,<;_ to find inhibitor candidates of PfENR by using I igands from the natural compound database of Medicinal Plants in Indonesia. On the GOLD software moleculer docking experiments were perfom1ed between ligands and macromolecule target PfENR. This target that has been optimized with residue removal and charges addition. Ligand is expected to be the PfENR inhibitors. Based on the results obtained from the in silico screening there were S inhibitor candidates which expected to be developed as an antimalarials. These compounds \\"ere Kacmpferol 3-rhamnosyl-(1-3)-rhamnosyl- (1-6)-glucoside, Cyanidin 3.5-di-(6-1mlonylglucoside), 8-Hydroxyapigenin 8-(2",4"-disulfatoglucuronidc). Epigallocmechin 3.5.-di-O-gallate, a··;d Querceti.r1 3.4'-dimethyl ether 7-alpha-L- Arabinofuranosyl-(1-6)-glucoside with the GoldScore ranged from 80,63 to I 00,4 I.