

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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Abstrak

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 development 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 Plasmodium falciparum Enoyl Acyl Carrier Protein Reductase (PFENR). Inhibition of this enzyme cause the fatty acid biosynthesis type II will be terminated. In this research, in silica screening was performed using GOLD software, to find inhibitor candidates of PFENR by using ligands from the natural compound database of Medicinal Plants in Indonesia. On the GOLD software molecular docking experiments were performed 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 5 inhibitor candidates which expected to be developed as antimalarials. These compounds were Kacmpferol 3-rhamnosyl-(1-3)-rhamnosyl- (1-6)-glucoside, Cyanidin 3,5-di-(6-O-malonylglucoside), 8-Hydroxyapigenin 8-(2'',4''-disulfatoglucuronide). Epigallocatechin 3,5-di-O-gallate, and Quercetin 3,4'-dimethyl ether 7- α -L- Arabinofuranosyl-(1-6)-glucoside with the GoldScore ranged from 80,63 to 100,41.