Penapisan in silico antimalaria dari basis data tanaman obat Indonesia terhadap target plasmepsin = In silico screening of antimalarial from Indonesian medicinal plants database to plasmepsin target

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Abstrak

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Malaria merupakan salah satu penyakit yang menyebabkan korban jutaan jiwa setiap tahun. Plasmepsin adalah enzim utama di antara enzim lain dalam siklus hidup plasmodium penyebab malaria yang mendegradasi hemoglobin selama fase eritrosit di dalam vakuola makanan. Dewasa ini, industri farmasi telah berupaya untuk mengembangkan agen terapetik yang dapat menyembuhkan penyakit malaria melalui penemuan senyawa baru penghambat plasmepsin mengingat adanya penyebaran strain yang resisten terhadap obat antimalaria. Namun, karena biaya yang tinggi dan waktu yang lama, metode konvensional untuk penemuan obat baru yang dilakukan secara in vivo dan in vitro sulit terealisasikan sehingga para ilmuwan kemudian beralih kepada metode baru yaitu penapisan in silico. Jenis penapisan in silico yang akan dilakukan dalam penelitian ini adalah penapisan berbasis struktur dengan menggunakan Basis Data Tanaman Obat Indonesia dan perangkat lunak GOLD. Berdasarkan penapisan ini, didapatkan hasil 11 kandidat senyawa inhibitor yang diharapkan dapat dikembangkan sebagai obat antimalaria. Senyawa tersebut yaitu Trimyristin; Cyanidin 3,5-di-(6-malonylglucoside); Isoscutellarein 4?-methyl ether 8-(6?-n-butylglucuronide); Cyanidin 3-(6?-malonylglucoside)-5-glucoside; Multifloroside; Delphinidin 3-(2-rhamnosyl-6-malonylglucoside); Delphinidin 3-(6-malonylglucoside)-3?,5?-di-(6-p-coumaroylglucoside); Cyanidin 3-[6-(6-sinapylglucosyl)-2-xylosylgalactoside; Kaempferol 3-glucosyl-(1-3)-rhamnosyl-(1-6)-galactoside; Sanggenofuran A; dan Lycopene dengan kisaran GOLDScore dari 78,4647 sampai 98,2836. Dua kandidat di antaranya berikatan dengan seluruh residu dari sisi katalitik plasmepsin yaitu Asp34 dan Asp214.
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ABSTRACT
<i>Malaria is one of diseases that annually emerge millions victim. Among the other enzymes, plasmepsin is the main enzyme in plasmodium life cycle that degrades hemoglobin during erythrocytic phase in food vacuole. Recently, pharmaceutical industries have been trying to develop therapeutic agents that be able to cure malaria through discovery of new plasmepsin inhibitor compounds, regarding to the spread of drug-resistant strains for antimalarial. However, due to high cost and long term, conventional methods for discovery of new drugs that were done in vivo and in vitro were difficult to be realized so that the scientists then shift to the

new method called in silico screening. The chosen in silico screening method in this experiment is structure-based screening by using GOLD software and Indonesian Medicinal Plants Database. Based on the obtained results from this screening, there are 11 inhibitor candidates which are expected to be developed as antimalarial. These compounds are Trimyristin; Cyanidin 3,5-di-(6-malonylglucoside); Isoscutellarein 4?-methyl ether 8-(6?-n-butylglucuronide); Cyanidin 3-(6?-malonylglucoside)-5-glucoside; Multifloroside; Delphinidin 3-(2-rhamnosyl-6-malonylglucoside); Delphinidin 3-(6-malonylglucoside)-3?,5?-di-(6-p-coumaroylglucoside); Cyanidin 3-[6-(6-sinapylglucosyl)-2-xylosylgalactoside; Kaempferol 3-glucosyl-(1-3)-rhamnosyl-(1-6)-galactoside; Sanggenofuran A; and Lycopene with GOLDScore range from 78,4647 to 98,2836. Two of them bind with all residues in catalytic site of plasmepsin which are Asp34 and Asp214.</i>