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In silico screening of anti-malarial from Indonesian medicinal plants database to plasmepsin target

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Malaria is one of diseases that annually emerge millions victim. Among the other enzymes, plasmepsin is the main enzyme in plasmodium life cycle which degrades hemoglobin during erythrocytic phase in food vacuole. Recently, pharmaceutical industries have been trying to develop therapeutic agents that are able to cure malaria through discovery of new plasmepsin inhibitor compounds. One of the developing approaches is *in silico* method. 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 anti-malarial. 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 GOLD Score range from 78,4647 to 98,2836. Two of them bind with all residues in catalytic site of plasmepsin which are Asp34 and Asp214.

Biography

Eko Aditya Rifai completed his Bachelor degree of Pharmacy and professional degree of pharmacist in University of Indonesia from 2007-2013. He is now a Master student of Bioinformatics at University of Glasgow, UK, starting from 2014. His research interests are in using the computational methods to discover potential inhibitors of enzymes correlated in human diseases, including drug design and molecular dynamics.

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