Analisis in silico turunan kurkumin baru pada enzim target antimalaria menggunakan autodock = In silico analysis of new curcumin derivates on target enzymes as antimalaria with autodock / Antonius Julio Falian

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Abstrak

[ABSTRAK
Malaria merupakan salah satu penyakit yang sering terjadi di negara tropis dan subtropis. Penyakit malaria banyak terjadi di sebagian besar wilayah Indonesia, seperti Irian Jaya, Nusa Tenggara Barat (NTB) dan Nusa Tenggara Timur (NTT). Berdasarkan data terakhir WHO pada tahun 2013, tercatat sebanyak 198 juta kasus malaria di seluruh dunia, dengan jumlah kematian sebanyak 584.000 jiwa. Pengobatan yang pernah ada untuk jenis malaria Plasmodium falciparum adalah klorokuin, sulfadoksin – pirimetamin, kinin, meflokuin dan artemisinin. Akan tetapi, meningkatnya resistensi parasit pada obat antimalaria, melemahkan upaya pengendalian malaria. Penambatan molekuler sebagai salah satu metode pendekatan in silico telah digunakan pada pencarian senyawa berkhasiat untuk menangani malaria. Dalam satu dekade terakhir, diketahui bahwa senyawa turunan kurkumin memiliki efek sinergis dengan artemisinin terhadap Plasmodium berghei secara in vivo. Pada penelitian ini, dilakukan penambatan molekuler senyawa turunan kurkumin baru terhadap enzim target antimalaria. Penambatan dilakukan menggunakan piranti lunak AutoDock. Berdasarkan hasil penambatan, didapatkan senyawa terbaik yang berpotensi sebagai obat antimalaria baru, yang dapat menyerang di sisi aktif tertentu dari Plasmodium falciparum, yaitu : 1,4-dihidrodiazepin-6-morfolinometil kurkumin pada enzim PfDHFR dan Pirimidin-2-on-5-morfolinometil kurkumin pada enzim PfDHODH.
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ABSTRACT
Malaria is a disease that often occurs in tropical and subtropical countries. Prevalent of malaria in most parts of Indonesia, such as Irian Jaya, West Nusa Tenggara (NTB) and East Nusa Tenggara (NTT). Based on the WHO's last data in 2013, there were 198 million cases of malaria worldwide, with the number of deaths by 584,000 inhabitants. Treatment for this type of Plasmodium falciparum malaria is chloroquine, sulfadoxine - pyrimethamine, quinine, mefloquine and artemisinin. However, increasing parasite resistance to the antimalarial drug, making malaria control efforts become effortless. Molecular docking as one method in silico approaches have been used in the search for efficacious compounds addressing malaria. In the last decade, it is known that the compound curcumin analogues have synergistic effect with artemisinin against Plasmodium berghei in vivo. In this study, we employed docking of new molecular compounds

curcumin derivates as antimalarial target enzymes. Molecular docking is performed using Autodock. Based on the docking result, best compound is obtained as a potential new antimalarial drug, which can be attacked in certain active side of Plasmodium falciparum, which is 1,4-dihydrodiazepin-6-morpholinomethyl curcumin on PfDHFR enzyme dan Pyrimidin-2-one-5-morpholinomethyl curcumin on PfDHODH enzyme., Malaria is a disease that often occurs in tropical and subtropical countries.

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