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[Abstract ID: ABS-85]

Molecular Docking Studies of Potential Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside as Inhibitor antiMalaria

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Abstract

The aims of this research is to analysis the potential Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside as an inhibitor Plasmodium falciparum Enoyl Acyl Carrier Protein Reductase (PfENR) compound for antimalaria. The method used to analysis the potential Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside as an antimalaria was insilico approach by molecular docking using Autodock Vina. Based on the free energy parameter analized , the value of free energy is -11.6 kcal /mol with 5 repetisions. The free energy value from the analysis results was quite low, this means that Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside is stable to be used as an inhibitor of Plasmodium falciparum Enoyl Acyl Carrier Protein Reductase (PfENR). Because the lower the free energy of a molecule the more stable the molecule. Based on hydrogen bond parameters, there were hydrogen bonds in Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside and PfENR receptors. This shows that Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside binding PfENR receptors to strong and stable. Based on the parameters of the analysis of Ligand and Receptor Interactions also showed that Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside compounds were stable used as Plasmodium falciparum Enoyl Acyl Carrier Protein Reductase (PfENR inhibitors for antimalaria. **(Approx. 190 words)**

Keywords: docking; inhibitor; Quercetin; antimalaria;

Topic: Physics related sciences

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2	**[ABS-85 PAYMENT_PROOF] Molecular Docking Studies of Potential Quercetin 3,4-dimethyl ether 7-alpha-LArabinofuranosyl-(1-6)-glucoside as Inhibitor antiMalaria** *Nya Daniaty Malau (a*), S T Azzahra (b)* **Server time** : Tuesday, 10 September 2019 - 08:41:51 **File** : payment_proof (File ID 139, image/jpeg: 74.0 kb) **Topic** : Physics related sciences **Paid amount** : IDR 3 million **(Make sure that it is correct)** **Payment date** : 2019.09.10 **(Make sure that it is correct)** **Info** :
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