SINTESIS DAN PENAMBATAN MOLEKUL SENYAWA ANALOG KURKUMIN MONOKARBONIL ASIMETRIS SEBAGAI ANTIMALARIA

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INTISARI

Telah dilakukan penelitian berjudul Sintesis dan Penambatan Molekul Senyawa Analog Kurkumin Monokarbonil Asimetris Sebagai Antimalaria. Penelitian bertujuan melakukan sintesis senyawa analog kurkumin monokarbonil asimetris (**AKMA**) dari senyawa vanilidinaseton serta melakukan uji *in-silico* antimalaria melalui penambatan molekul dan profil ADMET.

Sintesis senyawa **AKMA** diperoleh dari reaksi aldol kondensasi antara vanilidinaseton dengan turunan benzaldehid (2-hidroksibenzaldehid dan 2-hidroksi-3-metoksibenzaldehida) menggunakan katalis HCl 3N. Vanilidinaseton diperoleh dari reaksi kondensasi vanilin dan aseton dengan bantuan katalis NaOH 10%. Hasil dielusidasi dengan FT-IR, LC-MS dan ^{1}H-NMR. Penambatan molekul antimalaria dilakukan menggunakan *software autodock4* antara **AKMA** dengan protein PfDHFR-TS.

Senyawa (1E,4E)-1-(4-hidroksi-3-metoksifenil)-5-(2-hidroksifenol)penta-1,4-dien-3-on (**AKMA A**) dan (1E,4E)-1-(2-hidroksi-3-metoksifenil)-5-(4-hidroksi-3-metoksifenil)penta-1,4-dien-3-on (**AKMA B**) berhasil disintesis dengan rendemen 27,5% dan 34,35%. Penambatan molekul **AKMA A** dan **AKMA B** diperoleh nilai afinitas ikatan yg lebih rendah (-7,39 dan -7,25 kkal/mmol) dibandingkan ligan native (-5,81 kkal/mmol), vanilidinaseton (-6,14 kkal/mmol), dan kurkumin (-7,14 kkal/mmol). Hasil analisis ADMET menunjukkan senyawa **AKMA A** dan **AKMA B** merupakan kandidat obat oral.

Kata kunci : Antimalaria, Kurkumin asimetris, Penambatan molekul

SYNTHESIS AND MOLECULAR DOCKING OF ASYMMETRIC MONO-CARBONYL CURCUMIN ANALOGUES AS AN ANTIMALARIA

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ABSTRACT

The experiment of Synthesis and Docking Molecular of Asymmetric monocarbonyl Curcumin Analogues as An Antimalaria has been carried out. The aim of this study was to synthesize asymmetric monocarbonyl curcumin analogues **(AKMA)** from vanillydenacetone and *in-silico* antimalarial study using molecular penambatan & ADMET profile.

The synthesis of **AKMA** was obtained from the aldol condensations reaction between vanilydenacetone with benzaldehyde derivatives (2-hidroxybenzaldehyde and 2-hidroxy-3-methoxybenzaldehyde) with using HCL 3N as a catalyst. Vanilydenacetone was obtained from condensation reaction between vanilin and acetone using NaOH 10% as a catalyst. The result was elucidated with FT-IR, LC-MS, and ^{1}H-NMR. Penambatan molecular was carried out with using software autodock4 between **AKMA** with PfDHFR-TS protein.

The (1E,4E)-1-(4-hydroxy-3-methoxyphenyl)-5-(2-hydroxyphenyl)penta-1,4-dien-3-one (**AKMA A**) and (1E,4E)-1-(2-hydroxy-3-methoxyphenyl)-5-(4-hydroxy-3-methoxyphenyl)penta-1,4-dien-3-one (**AKMA B**) were succesfully synthesized with yield of 27,5 % and 34,35% respectively. Molecular penambatan studies **AKMA A** and **AKMA B** showed lower bond affinity (-7,39 dan -7,25 kkal/mmol) compared to native ligand (-5,81 kkal/mmol), vanillydenacetone (-6,14 kkal/mmol), curcumin (-7,14 kkal/mmol). The result of ADMET analysis showed that **AKMA A** and **AKMA B** were oral drug candidate.

Keyword : Antimalarial. Assymetric curcummine, Molecular docking