DESAIN DAN SINTESIS SENYAWA ANALOG MONOKARBONIL KURKUMIN ASIMETRIS SEBAGAI SENYAWA ANTIMALARIA

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INTISARI

Desain dan sintesis senyawa analog monokarbonil kurkumin asimetris (AMKA) sebagai senyawa antimalaria telah dilakukan. Desain senyawa antimalaria dilakukan melalui penambatan molekul terhadap protein PfDHFR-TS dan analisis ADMET terhadap senyawa analog monokarbonil kurkumin asimetris (AMKA). Sintesis senyawa AMKA dilakukan melalui reaksi kondensasi *Claisen-Schimdt* terhadap senyawa benzalaseton dengan turunan benzaldehid. Benzalaseton disintesis dari reaksi kondensasi *Claisen-Schmidt* vanilin atau o-vanilin dengan aseton menggunakan katalis NaOH 8 %. Elusidasi struktur produk dilakukan menggunakan spektrometer FTIR, GC-MS, ^{1}H NMR dan ^{13}C-NMR.

Penambatan molekul menghasilkan tiga senyawa AMKA yang memiliki interaksi dengan tingkat energi terendah yakni AMKA A -7,83 kkal/mol, AMKA D -7,31 kkal/mol dan AMKA E -7,90 kkal/mol. AMKA A, D dan E memiliki profil ADMET yang lebih baik sebagai senyawa obat oral dibandingkan dengan kurkumin. Sintesis **AMKA A**, **D** dan **E** berhasil dilakukan melalui senyawa intermediat benzalaseton **A** dan benzalaseton **B** dengan rendemen berturut-turut 91,3; 67,8 dan 74,1 %.

Kata Kunci: ADMET, AMKA, Antimalaria, penambatan molekul.

DESIGN AND SYNTHESIS OF ASSYMETRIC MONOCARBONYL CURCUMIN ANALOGUES AS ANTIMALARIA COMPOUNDS

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ABSTRACT

Design and synthesis of an asymmetric monocarbonyl analogue of curcumin (AMKA) as an antimalarial compound have been carried out. The design of the antimalarial compound was carried out by molecular docking using PfDHFR-TS as protein target and ADMET analysis of the AMKA. The synthesis of AMKA was carried out through a Claisen-Schimdt condensation reaction of benzalacetone with benzaldehyde derivatives. Benzalacetone is synthesized from the Claisen-Schmidt condensation reaction of vanillin or o-vanillin with acetone using 8 % NaOH as a catalyst. The structure elucidation of the product was carried out using FTIR, GC-MS, ^{1}H NMR and ^{13}C-NMR spectrometers.

Molecular docking resulted three proposed **AMKA** compounds having the lowest affinity interactions, **AMKA A** -7.83 kcal/mol, **AMKA D** -7.31 kcal/mol and **AMKA E** -7.90 kcal/mol, respectively. **AMKA A, D** and **E** had a better ADMET analysis as an oral drug compound compared to curcumin. The synthesis of **AMKA A, D** and **E** was successfully carried out through the benzalacetone A and benzalacetone B with yields of 91.3, 67.8 and 74.1 % respectively.

Keywords: ADMET, AMAC, antimalarial, molecular docking.