SINTESIS BEBERAPA SENYAWA ANALOG KURKUMIN SEBAGAI SENYAWA ANTIMALARIA TERHADAP PLASMODIUM FALCIPARUM DAN PENAMBATAN MOLEKULER TERHADAP PROTEIN PfAPT6

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INTISARI

Sintesis senyawa analog kurkumin 2,6-*bis*(3-hidroksibenzaliden) sikloheksanon (A); 2,6-*bis*(3-hidroksibenzaliden)siklopentanon (B); dan 2,6-*bis*(3-hidroksifenil)penta-1,4-diena-3-on (C) telah berhasil dilakukan. Sintesis senyawa analog kurkumin tersebut dilakukan menggunakan metode reaksi Claisen-Schmidt, mereaksikan 3-hidroksibenzaldehida dengan sikloheksanon, siklopentanon, dan aseton menggunakan pelarut THF dan katalis HCl 37%. Elusidasi struktur senyawa produk dianalisis dengan KLT, *TLC scanner*, spektrofotometer FTIR, ^{1}H-NMR, ^{13}C-NMR, dan LC-MS/MS. Uji aktivitas antiplasmodium diuji secara *in vitro* terhadap *Plasmodium falciparum* 3D7, dilanjutkan dengan kajian interaksi penambatan molekuler terhadap protein PfATP6.

Hasil sintesis senyawa 2,6-*bis*(3-hidroksibenziliden)sikloheksanon; 2,6-*bis*(3-hidroksibenziliden)siklopentanon; dan 1,5-*bis*(3-hidroksifenil)penta-1,4-diena-3-on diperoleh persentase hasil produk berturut-turut sebesar 78,87%; 53,44%; dan 64,16%. Hasil uji antiplasmodium senyawa analog kurkumin A, B, dan C diperoleh nilai IC_{50} menggunakan analisis probit SPSS dengan taraf signifikansi 95% berturut-turut sebesar 16,93; 31,88; dan 39,04 μM. Berdasarkan penambatan molekuler, diperoleh nilai afinitas ikatan berturut-turut sebesar -8,5; -8,4; dan -8,1 kkal/mol.

Kata kunci: 3-hidroksibenzaldehida, antiplasmodium, penambatan molekuler, sintesis

SYNTHESIS OF SEVERAL CURCUMIN ANALOGUES AS ANTIMALARIAL AGENT AGAINST PLASMODIUM FALCIPARUM AND MOLECULAR DOCKING TARGETING PfATP6 PROTEIN

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ABSTRACT

Synthesis of curcumin analogues 2,6-*bis*(3-hydroxybenzylidene) cyclohexanone (A); 2,6-*bis*(3-hydroxybenzylidene)cyclopentanone (B), and 1.5-*bis*(3-hydroxyphenyl)penta-1,4-diene-3-on (C) have been successfully accomplished. Synthesis of the curcumin analogues was carried out by condensation Claisen-Schmidt between 3-hidroxybenzaldehyde with cyclohexanone, cyclopentanone, and acetone, respectively. These curcumin analogues compound were characterized by TLC, TLC scanner, FTIR spectrophotometer ^{1}H-NMR, ^{13}C-NMR, and LC-MS/MS. Antimalarial activity of the analog compounds was tested by antiplasmodium assay of *Plasmodium falciparum* 3D7 and the results were evaluated the interaction and affinity bonding by molecular docking.

The spectroscopy characterization show that the reaction have been succesfully produce 2,6-*bis*(3-hydroxybenzylidene)cyclohexanone; 2,6-*bis*(3-hydroxybenzylidene)cyclopentanone, and 1.5-*bis*(3-hydroxyphenyl)penta-1,4-diene-3-on with yield of 78.87, 53.44, dan 64.16%, respectively. The IC_{50} value, represent against *P. falciparum* of the curcumin analogues were at IC_{50} 16.93, 31.88, and 39.04 μM, respectively. Then, based on compound A, B, and C were calculated by molecular docking, it was obtained that the value of affinity bonding -8.5, -8.4, dan -8.1 kkal/mol, respectively.

Keywords: 3-hidroxybenzaldehyde, antiplasmodium, molecular docking, synthesis