SINTESIS DAN PENAMBATAN MOLEKUL SENYAWA ANALOG KURKUMIN MONOKETON BERBAHAN DASAR SINAMALDEHIDA DAN 1-METIL-4-PIPERIDON SERTA UJI SITOTOKSISITAS TERHADAP SEL KANKER PAYUDARA MCF-7

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INTISARI

Penelitian sintesis dan penambatan molekul senyawa analog kurkumin monoketon berbahan dasar sinamaldehida dan 1-metil-4-piperidon serta uji sitotoksisitas terhadap sel kanker payudara MCF-7 telah berhasil dilakukan. Tahapan pertama penelitian ini adalah sintesis senyawa analog kurkumin monoketon secara eksperimental. Elusidasi struktur senyawa hasil sintesis dilakukan menggunakan ATR-IR, ^{1}H-NMR, dan ^{13}C-NMR. Pada penelitian ini dilakukan penambatan molekul menggunakan AutodockVina terhadap senyawa analog kurkumin monoketon dan kurkumin untuk memprediksi peran regulasinya terhadap 3 protein target yaitu Erα, PI3K, dan Bcl-2. Uji aktivitas antikanker senyawa analog kurkumin dilakukan secara *in vitro* terhadap sel kanker payudara MCF-7 melalui metode MTT.

Sintesis senyawa analog dilakukan dengan mereaksikan sinamaldehida dengan 1-metil-4-piperidon melalui reaksi kondensasi Claisen-Schmidt. Produk yang dihasilkan berupa padatan berwarna kuning dengan persen hasil sebesar 60,14%. Hasil penambatan molekul menunjukkan nilai afinitas ikatan senyawa analog kurkumin dengan protein Erα, Bcl-2, dan PI3K secara berturut-turut adalah -8,2; -9,4; dan -7,7 kkal/mol, sedangkan nilai afinitas ikatan senyawa kurkumin dengan protein Erα, PI3K, dan Bcl-2 yaitu -7,8 kkal/mol. Pengujian aktivitas antikanker senyawa analog kurkumin monoketon terhadap sel kanker payudara MCF-7 menghasilkan nilai IC_{50} sebesar 906,93 μg/mL, yang dikategorikan tidak toksik atau kurang potensial untuk dijadikan senyawa antikanker.

Kata kunci: Analog kurkumin, antikanker, MCF-7, penambatan molekul, sinamaldehida.

SYNTHESIS AND MOLECULAR DOCKING OF MONOKETONE CURCUMIN ANALOGUE COMPOUND FROM CINNAMALDEHYDE AND 1-METHYL-4-PIPERIDONE AND CYTOTOXICITY ASSAY AGAINST MCF-7 BREAST CANCER CELL LINE

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ABSTRACT

The experiment of synthesis and molecular docking of monoketone curcumin analog compound from cinnamaldehyde and 1-methyl-4-piperidone and cytotoxicity assay against MCF-7 breast cancer cell had been carried out. The first step of this study involved the experimental synthesis of monoketone curcumin analog. The product was elucidated using ATR-IR, ^{1}H-NMR, and ^{13}C-NMR. In this study, molecular docking of curcumin analog compound and curcumin was carried out to predict their regulatory role against three target proteins, namely Erα, PI3K, and Bcl-2. The *in vitro* cytotoxicity test of curcumin analog was performed against MCF-7 breast cancer cell using MTT method.

The curcumin analog was obtained by reacting cinnamaldehyde and 1-methyl-4-piperidone via Claisen-Schmist condensation reaction and was produced in 60,14% yields. The results of molecular docking showed that the binding affinity of curcumin analog compound to Erα, Bcl-2, and PI3K were -8,2; -9,4; dan -7,7 kcal/mol, respectively. Meanwhile, the binding affinity values of curcumin with the proteins Erα, PI3K, and Bcl-2 were -7.8 kcal/mol. Testing the anticancer activity of curcumin analog compound against MCF-7 showed inactive activity or less potents to be considered as an anticancer compound with an IC_{50} of 906,93 μg/mL.

Keywords: Anticancer, cinnamaldehyde, curcumin analogue, MCF-7, molecular docking.