SINTESIS SENYAWA ANALOG KURKUMIN MONOKARBONIL BERBAHAN DASAR *p*-DIMETILAMINOBENZALDEHIDA, PENAMBATAN MOLEKUL TERHADAP VARIASI PROTEIN, SERTA SITOTOKSISITAS TERHADAP SEL KANKER PAYUDARA T47D

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INTISARI

Penelitian mengenai sintesis senyawa analog kurkumin monokarbonil berbahan dasar *p*-dimetilaminobenzaldehida, penambatan molekul terhadap variasi protein, serta uji sitotoksisitas terhadap sel kanker payudara T47D bertujuan untuk melakukan sintesis, mengetahui afinitas ikatan dan interaksi analog kurkumin dengan protein target melalui penambatan molekuler, serta mengetahui sitotoksisitasnya pada sel kanker payudara T47D dan sel normal Vero. Senyawa analog kurkumin disintesis melalui reaksi kondensasi aldol Claisen-Schmidt pada suasana basa. Karakterisasi produk dilakukan dengan ATR-IR, spektroskopi ^{1}H-NMR, dan ^{13}C-NMR. Penambatan molekuler analog kurkumin dilakukan terhadap protein EGFR, Bcl-2, dan p53 mutan. Metode *Microculture Tetrazolium Technique* (MTT) dipilih dalam uji sitotoksisitas kurkumin dan analog kurkumin terhadap sel kanker payudara T47D dan sel normal Vero.

Berdasarkan hasil sintesis diperoleh senyawa analog kurkumin berwarna oranye dengan persen hasil sebesar 91%. Penambatan molekuler terhadap protein EGFR dan p53 mutan menghasilkan afinitas ikatan analog kurkumin tertinggi sedangkan pada protein Bcl-2 afinitas ikatan analog kurkumin lebih rendah dibandingkan ligan asli. Hasil uji *in vitro* sitotoksisitas menunjukkan senyawa analog kurkumin dan kurkumin memiliki sitotoksisitas sangat tinggi dengan nilai IC_{50} 6,75 dan 5,41 µg/mL terhadap sel kanker payudara T47D, kedua senyawa tersebut memiliki indeks selektivitas tinggi terhadap sel normal Vero.

Kata kunci: analog kurkumin, *p*-dimetilaminobenzaldehid, penambatan molekuler, uji sitotoksisitas.

SYNTHESIS OF MONOCARBONYL CURCUMIN ANALOG COMPOUND FROM p-DIMETHYLAMINOBENZALDEHYDE, MOLECULAR DOCKING ON VARIOUS PROTEINS, AND CYTOTOXICITY AGAINST T47D BREAST CANCER CELL

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ABSTRACT

Research on the synthesis of monocarbonyl curcumin analog compounds based on *p*-dimethylaminobenzaldehyde, molecular docking against various proteins, and cytotoxicity assay on T47D breast cancer cells aimed to synthesize the compounds, investigate the binding affinity and interactions of curcumin analogs with target proteins through molecular docking, and evaluate their cytotoxic effects on T47D breast cancer cells and normal Vero cells. The curcumin analog compound was synthesized via a base-catalyzed Claisen–Schmidt aldol condensation reaction. Product characterization was carried out using ATR-IR, ^{1}H-NMR, and ^{13}C-NMR spectroscopy. Molecular docking of the curcumin analog was performed against EGFR, Bcl-2, and mutant p53 proteins. The Microculture Tetrazolium Technique (MTT) method was selected to assess the cytotoxicity of curcumin and its analogs toward T47D breast cancer cells and normal Vero cells.

Based on the synthesis results, an orange-colored curcumin analog compound was obtained with a yield of 91%. Molecular docking against EGFR and mutant p53 proteins showed the highest binding affinity for the curcumin analog, whereas docking against the Bcl-2 protein revealed a lower affinity compared to the native ligand. In vitro cytotoxicity assay results demonstrated that both the curcumin analog and curcumin exhibited very high cytotoxicity toward T47D breast cancer cells, with IC_{50} values of 6.75 and 5.41 µg/mL Both compounds also showed high selectivity toward normal Vero cells.

Keywords: curcumin analog, cytotoxicity assay, molecular docking, *p*-dimethylaminobenzaldehyde.

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