

**SINTESIS DAN PENAMBATAN MOLEKUL ANALOG KURKUMIN  
DARI 2-HIDROKSIBENZALDEHIDA DENGAN  
N-BENZIL-4-PIPERIDON SERTA AKTIVITAS SITOTOKSIKNYA  
TERHADAP SEL KANKER PAYUDARA T47D**

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**INTISARI**

Sintesis dan penambatan molekul analog kurkumin dari bahan 2-hidroksibenzaldehida dengan *N*-benzil-4-piperidon serta aktivitas sitotoksiknya terhadap sel kanker payudara T47D telah dilakukan. Analog kurkumin disintesis melalui reaksi kondensasi aldol Claisen-Schmidt dalam etanol menggunakan katalis NaOH 40% (b/v) dan metode sonikasi. Hasil sintesis dikarakterisasi menggunakan instrumen KLT *Scanner*, ATR-IR, spektroskopi <sup>1</sup>H-NMR, dan <sup>13</sup>C-NMR. Penambatan molekul pada kurkumin dan analog kurkumin dilakukan terhadap variasi protein yaitu EGFR, Bcl-2, dan p53 mutan. Uji sitotoksitas kurkumin dan analog kurkumin dilakukan menggunakan metode MTT terhadap sel kanker payudara T47D dan sel normal Vero.

Reaksi kondensasi aldol menghasilkan analog kurkumin berwujud padatan, berwarna oranye dengan persen hasil 93%, dan titik leleh 141,9-144,2 °C. Hasil penambatan molekul menunjukkan bahwa analog kurkumin dapat berikatan dengan sisi aktif protein EGFR, Bcl-2, dan p53 mutan dan menunjukkan nilai afinitas pengikatan yang lebih rendah dibandingkan dengan kurkumin. Hasil uji sitotoksitas terhadap sel kanker payudara T47D dan sel normal Vero menunjukkan nilai IC<sub>50</sub> masing-masing 44,85 dan 961,06 µg mL<sup>-1</sup>. Sementara itu, kurkumin menunjukkan nilai IC<sub>50</sub> masing-masing 10,60 dan 16,23 µg mL<sup>-1</sup>. Perhitungan indeks selektivitas menunjukkan bahwa analog kurkumin memiliki selektivitas yang tinggi dengan nilai 21,43 dan lebih baik dari kurkumin yang memiliki selektivitas yang sedikit selektif dengan nilai 1,53.

Kata kunci: analog kurkumin, kondensasi aldol, kurkumin, penambatan molekul.

***SYNTHESIS AND MOLECULAR DOCKING OF CURCUMIN ANALOG  
FROM 2-HYDROXYBENZALDEHYDE WITH N-BENZYL-4-PIPERIDONE  
AND ITS CYTOTOXIC ACTIVITY AGAINST T47D BREAST CANCER CELL***

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**ABSTRACT**

Synthesis and molecular docking studies of a curcumin analog derived from 2-hydroxybenzaldehyde with N-benzyl-4-piperidone, along with its cytotoxic activity against T47D breast cancer cell, have been conducted. The curcumin analog was synthesized through a Claisen-Schmidt aldol condensation reaction in ethanol using a 40% (m/v) NaOH catalyst and the sonication method. The product was characterized using a KLT Scanner, ATR-IR, <sup>1</sup>H-NMR, and <sup>13</sup>C-NMR spectroscopy. Molecular docking studies of curcumin and curcumin analog were carried out on various proteins, namely EGFR, Bcl-2, and mutant p53 proteins. The cytotoxicity of the curcumin and curcumin analog was evaluated using the MTT assay against breast cancer T47D cell and normal Vero cell.

The aldol condensation reaction produced curcumin analog as orange solids with a 93% yield and a melting point of 141.9-144.2 °C. Molecular docking studies indicated that the curcumin analog could bind to the active side of EGFR, Bcl-2, and mutant p53 proteins, showing lower binding affinity values compared to curcumin. Cytotoxic assay against T47D breast cancer cell and normal Vero cell revealed IC<sub>50</sub> values of 44.85 and 961.06 µg mL<sup>-1</sup>, respectively. Meanwhile, curcumin showed IC<sub>50</sub> values of 10.60 and 16.23 µg mL<sup>-1</sup> respectively. The selectivity index calculation demonstrated that the curcumin analog possesses high selectivity, with a value of 21.43 and is better than curcumin which has a slightly selective selectivity with the value of 1.53.

Keywords: aldol condensation, analog curcumin, curcumin, molecular docking.