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**Sintesis Nanosuspensi Analog Kurkumin Berbahan Dasar 4-Dimetilaminobenzaldehida, Uji Sitotoksisitas,
dan Penambatan Molekul sebagai Kandidat Senyawa Antikanker Payudara**
Salma Putri Nursafira, Dr. Endang Astuti, M.Si. ; Dr. Deni Pranowo, S.Si., M.Si.
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SINTESIS NANOSUSPENSI ANALOG KURKUMIN BERBAHAN DASAR 4-DIMETILAMINOBENZALDEHIDA, UJI SITOTOKSISITAS, DAN PENAMBATAN MOLEKUL SEBAGAI KANDIDAT SENYAWA ANTIKANKER PAYUDARA

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INTISARI

Penelitian mengenai sintesis nanosuspensi analog kurkumin berbahan dasar 4-dimetilaminobenzaldehida, uji sitotoksisitas, dan penambatan molekul sebagai kandidat senyawa antikanker payudara telah dilakukan. Penelitian ini bertujuan untuk melakukan sintesis, membuat formulasi nanosuspensi, mengetahui afinitas ikatan, dan interaksi analog kurkumin dengan protein target melalui penambatan molekuler, serta mengetahui sitotoksisitas terhadap sel kanker payudara MCF-7 dan sel normal (Vero). Senyawa analog kurkumin disintesis melalui reaksi kondensasi aldol Claisen–Schmidt pada suasana basa. Formulasi nanosupensi analog kurkumin dilakukan dengan metode penguapan pelarut menggunakan pelarut diklorometana dengan penambahan surfaktan Tween 60. Karakterisasi produk dilakukan dengan instrumen *Attenuated Total Reflectance–Infrared* (ATR-IR), *Proton Nuclear Magnetic Resonance* (^{1}H NMR), dan *Carbon-13 Nuclear Magnetic Resonance* (^{13}C NMR). Karakterisasi hasil nanosuspensi dilakukan dengan *Scanning Electron Microscopy* (SEM) dan *Particle Size Analysis* berbasis *Dynamic Light Scattering* (PSA-DLS). Penentuan aktivitas sitotoksik dilakukan dengan metode *Microculture Tetrazolium Technique (*MTT*)* terhadap sel kanker payudara MCF-7 dan sel normal (Vero). Hasil efek sitotoksik senyawa obat kemudian dikonfirmasi dengan penambatan molekuler terhadap protein Bcl-2, ER-α, dan PI3K.

Hasil sintesis berupa senyawa analog kurkumin berwarna oranye dengan kemurnian 100% dan persentase hasil 44,4%. Formulasi nanosuspensi analog kurkumin menghasilkan sediaan nanosuspensi yang homogen dan stabil dengan ukuran partikel 125 nm. Hasil uji *in vitro* menunjukkan senyawa analog kurkumin dan nanosuspensinya memiliki aktivitas sitotoksik terhadap sel kanker MCF-7 dengan nilai IC_{50} masing-masing 98,83 dan 133,77 μg mL^{-1}. Kedua senyawa tersebut lebih selektif daripada senyawa kurkumin dengan indeks selektivitas masing-masing 1,41 dan 13,11 terhadap sel normal (Vero). Penambatan molekuler analog kurkumin terhadap protein Bcl-2, ER-α, dan PI3K menghasilkan afinitas ikatan yang lebih rendah daripada kurkumin, serta menunjukkan interaksi spesifik dengan residu asam amino.

Kata kunci: analog kurkumin, antikanker, kondensasi aldol, nanosuspensi.

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SYNTHESIS OF CURCUMIN ANALOGUE NANOSUSPENSION BASED ON 4-DIMETHYLAMINOBENZALDEHYDE, CYTOTOXICITY TEST, AND MOLECULAR DOCKING AS A CANDIDATE FOR AN ANTI-BREAST CANCER COMPOUND

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ABSTRACT

Research on the synthesis of curcumin analogue nanosuspension based on 4-dimethylaminobenzaldehyde, cytotoxicity test, and molecular docking as a candidate for an anti-breast cancer compound was conducted. This research aimed to synthesize the curcumin analog compound, formulate it into a nanosuspension, determine its binding affinity and interactions with target proteins through molecular docking, and evaluate its cytotoxic activity against MCF-7 breast cancer cells and Vero cells. The curcumin analog was synthesized via a Claisen–Schmidt aldol condensation under basic conditions. The curcumin analog nanosuspension was formulated using the solvent evaporation method with dichloromethane as the solvent and Tween 60 as the surfactant. Product characterization was carried out using Attenuated Total Reflectance–Infrared (ATR-IR), Proton Nuclear Magnetic Resonance (^{1}H NMR), and Carbon-13 Nuclear Magnetic Resonance (^{13}C NMR). The nanosuspension was characterized using Scanning Electron Microscopy (SEM) and Particle Size Analysis based on Dynamic Light Scattering (PSA-DLS). Cytotoxic activity was determined using the Microculture Tetrazolium Technique (MTT) against MCF-7 breast cancer cells and Vero cells. The cytotoxic effect of the compound was then confirmed through molecular docking against Bcl-2, ER-α, and PI3K proteins.

The synthesis yielded an orange curcumin analog compound with 100% purity and a percentage yield of 44.4%. The formulation of the curcumin analog nanosuspension produced a homogeneous and stable nanosuspension with a particle size of 125 nm. The in vitro cytotoxicity test showed that the curcumin analog compound and its nanosuspension exhibited cytotoxic activity against MCF-7 cells, with IC_{50} values respectively of 98.83 and 133.77 μg mL^{-1}. Both compounds were more selective than curcumin against Vero cells, with selectivity index values respectively of 1.41 and 13.11. Molecular docking of the curcumin analog against Bcl-2, ER-α, and PI3K proteins resulted in lower binding affinity values than curcumin and showed specific interactions with amino acid residues.

Keywords: aldol condensation, anticancer, curcumin analog, nanosuspension.