ANALISIS POTENSI KANDIDAT ANTIKANKER DARI EKSTRAK KULIT POHON ANDALAS (*Morus macroura Miq.*) TERHADAP KANKER PAYUDARA MELALUI PENDEKATAN *NETWORK PHARMACOLOGY* DAN *MOLECULAR DOCKING*

Skripsi

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ABSTRACT

ANALYSIS OF THE POTENTIAL ANTICANCER CANDIDATES FROM ANDALAS TREE BARK EXTRACT (Morus macroura Miq.) AGAINST BREAST CANCER THROUGH A NETWORK PHARMACOLOGY AND MOLECULAR DOCKING APPROACH

By

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Breast cancer is the disease with the highest prevalence among women in Indonesia and worldwide. Limitations of conventional therapy, such as side effects and drug resistance, drive the need for alternative therapies based on natural products. The andalas tree (Morus macroura Miq.) is known to be rich in bioactive compounds, yet its anticancer potential against breast cancer through a multitarget approach is not widely studied. This study analyzes the anticancer candidate potential of andalas bark extract against breast cancer through network pharmacology and molecular docking.

This descriptive in silico study was conducted from July–October 2025 and May–August 2026 at InviLab Bogor and in Padang. Compounds were identified using LC-HRMS, then screened for drug-likeness, ADMET, toxicity, and biological activity. Network pharmacology was analyzed using SwissTargetPrediction, GeneCards, STRING, and Cytoscape; docking was performed using MOE against the top three hub genes from network pharmacology.

A total of 52 compounds were identified, of which 22 met all selection criteria. Network pharmacology identified 62 common targets, with STAT3, CTNNB1, and AKT1 as main hub genes associated with EGFR TKI resistance and pathways in cancer. Redocking showed an RMSD below 2Å, indicating a valid docking method. Macrourone C showed the best affinity toward STAT3 and AKT1, while Sorocein A showed the best affinity toward CTNNB1; both were computationally better than the comparator drugs.

Macrourone C and Sorocein A from andalas bark extract are showing potential to serve as candidate anticancer agents against breast cancer through an in silico approach. These findings are remaining predictive and are requiring further in vitro/in vivo validation before being concluded effective.

Keywords: *Breast cancer; Morus macroura; network pharmacology; molecular docking; STAT3; CTNNB1; AKT1*

ABSTRAK

ANALISIS POTENSI KANDIDAT ANTIKANKER DARI EKSTRAK KULIT POHON ANDALAS (*Morus macroura Miq.*) TERHADAP KANKER PAYUDARA MELALUI PENDEKATAN *NETWORK PHARMACOLOGY* DAN *MOLECULAR DOCKING*

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Kanker payudara merupakan kanker dengan prevalensi tertinggi pada perempuan di Indonesia dan dunia. Keterbatasan terapi konvensional, seperti efek samping dan resistensi obat, mendorong perlunya terapi alternatif berbasis bahan alam. Pohon andalas (*Morus macroura* Miq.) diketahui kaya senyawa bioaktif, namun potensi antikankernya terhadap kanker payudara melalui pendekatan multitarget belum banyak dikaji. Penelitian ini bertujuan menganalisis potensi kandidat antikanker dari ekstrak kulit pohon andalas terhadap kanker payudara melalui *network pharmacology* dan *molecular docking*.

Penelitian ini bersifat deskriptif *in silico*, dilaksanakan pada Juli–Oktober 2025 dan Mei–Agustus 2026 di InviLab Bogor dan Padang. Senyawa diidentifikasi menggunakan LC-HRMS, lalu diseleksi berdasarkan *drug-likeness*, ADMET, toksisitas, dan aktivitas biologis. *Network pharmacology* dianalisis menggunakan SwissTargetPrediction, GeneCards, STRING, dan Cytoscape; *molecular docking* dilakukan dengan MOE terhadap tiga *hub gene* teratas hasil *network pharmacology*.

Sebanyak 52 senyawa diidentifikasi, 22 di antaranya memenuhi seluruh kriteria seleksi. *Network pharmacology* menemukan 62 *common target*, dengan STAT3, CTNNB1, dan AKT1 sebagai *hub gene* utama yang diduga berperan pada jalur EGFR TKI resistance dan *pathways in cancer*. *Redocking* menunjukkan RMSD di bawah 2Å, sehingga metode docking dinyatakan valid. Macrourone C menunjukkan afinitas terbaik terhadap STAT3 dan AKT1, sementara Sorocein A terbaik terhadap CTNNB1, afinitas keduanya secara komputasional lebih baik dibanding obat pembanding.

Macrourone C dan Sorocein A dari ekstrak kulit pohon andalas berpotensi sebagai kandidat agen antikanker payudara melalui pendekatan *in silico*. Temuan ini bersifat prediktif dan memerlukan validasi *in vitro-in vivo* lanjutan sebelum disimpulkan sebagai agen antikanker efektif.

Kata Kunci: Kanker payudara; *Morus macroura*; *network pharmacology*; *molecular docking*; STAT3; CTNNB1; AKT1