

**UJI EFEK SINERGIS KOMBINASI MINYAK ATSIRI DAUN DAN BUAH
CENGKEH (*Syzygium aromaticum*) TERHADAP PENGHAMBATAN
RESEPTOR KANKER PAYUDARA : DOCKING MOLEKULER IN
SILICO DAN PENILAIAN TOKSISITAS MELALUI UJI BSLT**

ABSTRAK

Latar Belakang: Penggunaan senyawa bahan alam tunggal serta kemoterapi dalam pengobatan kanker masih memberikan dampak yang signifikan terhadap efek samping yang diberikan, diketahui minyak atsiri yang terkandung baik pada daun maupun buah cengkeh memiliki efek yang baik terhadap penghambatan berbagai jenis sel kanker. Potensi dari kombinasi keduanya diharapkan mampu berefek sinergis baik secara farmakologis terhadap penghambatan sel kanker payudara.

Tujuan Penelitian: Mengidentifikasi nilai binding affinity secara in silico pada senyawa eugenol dan eugenol asetat yang terkandung pada sampel terhadap reseptor kanker payudara, serta nilai toksisitas penggunaan tunggal dan kombinasi minyak atsiri daun dan buah cengkeh melalui pendekatan Brine shrimp lethality test.

Metode Penelitian: Senyawa aktif berupa ligan eugenol dan eugenol asetat dipreparasi menggunakan *discovery studio*, dan dilakukan docking menggunakan *pyrx*. Sampel minyak atsiri pada daun dan buah cengkeh ditarik menggunakan pelarut aquadest dengan metode destilasi uap, hasil kemudian dibuat beberapa pengenceran untuk nantinya diujikan pada larva udang (*Artemia salina*) dan dilakukan perhitungan persen mortalitas setelah 24 jam.

Hasil Penelitian: Hasil menunjukkan nilai *binding affinity* untuk eugenol (-5,7) dan eugenol asetat (-6,3) terhadap reseptor estrogen alfa, sedangkan pada reseptor HER2 (3PP0) untuk eugenol (-5,7) dan eugenol asetat (-6,0). Berdasarkan pengujian toksisitas diketahui nilai rata-rata LC50 pada 3 replikasi sampel yang diujikan untuk daun cengkeh tunggal (23,6 ppm), buah cengkeh tunggal (9,79 ppm), dan pada kombinasi perbandingan 50:50 yakni (24,92 ppm). Sehingga diketahui efek yang diberikan kombinasi secara in vivo belum dapat memberikan efek sinergis yang diharapkan dalam pengobatan terapi kanker.

Kata kunci: Daun cengkeh, buah cengkeh (*Syzygium aromaticum*), kombinasi, destilasi uap, in silico, toksisitas.

***SYNERGISTIC EFFECTS OF CLOVE LEAF AND FRUIT ESSENTIAL OIL
(*Syzygium aromaticum*) ON BREAST CANCER RECEPTOR INHIBITION :
IN SILICO MOLECULAR DOCKING AND TOXICITY ASSESSMENT VIA
BSLT TEST***

ABSTRACT

Background: The use of single natural compounds and chemotherapy in cancer treatment still has a significant impact on side effects. It is known that essential oils contained in both clove leaves and fruits have a positive effect on inhibiting various types of cancer cells. The potential of combining the two is expected to have a synergistic effect, both pharmacologically and in inhibiting breast cancer cells.

Research Objective: To identify the *binding affinity* of various eugenol and eugenol acetate compounds contained in the samples toward breast cancer receptors, as well as the toxicity values of single and combined use of clove leaf and fruit essential oils through the brine shrimp lethality test approach.

Research Method: Active compounds in the form of eugenol and eugenol acetate ligands were prepared using Discovery Studio, and docking was performed using Pyrx. Essential oil samples from clove leaves and fruits were extracted using aquadest solvent via steam distillation. The resulting extracts were diluted and tested on shrimp larvae (*Artemia salina*), with mortality rates calculated after 24 hours.

Research Results: The results showed binding affinity values for eugenol (-5.7) and eugenol acetate (-6.3) toward the estrogen receptor alpha, while for the HER2 receptor (3PP0), the values were -5.7 for eugenol and -6.0 for eugenol acetate. Based on toxicity testing, the average LC50 values for three replicates of the tested samples were 23.6 ppm for single clove leaves, 9.79 ppm for single clove fruits, and 24.92 ppm for the 50:50 combination. Thus, it was found that the combination did not produce the expected synergistic effect in vivo for cancer therapy.

Keywords: Clove leaves, clove fruit (*Syzygium aromaticum*), combination, steam distillation, in silico, toxicity.