

# Aktivitas Senyawa Geraniol Daun Kemangi (*Ocimum Americanum*) Terhadap Enzim *Muramidase A* dan *Glycosyltransferase P Streptococcus Sanguinis* Secara *In Silico*

## ABSTRAK

Daun kemangi *Ocimum americanum* telah terbukti mempunyai daya antibakteri terhadap bakteri Gram positif dan Gram negatif. Kandungan terbanyak dari *O. americanum* adalah terpenoid. Senyawa geraniol merupakan turunan dari terpenoid mempunyai persentase sebesar 37,70%. Bahan alam kemangi (*O. americanum*) diharapkan menjadi salah satu alternatif bahan obat kumur yang memiliki efek antibakteri terhadap biofilm *Streptococcus sanguinis*. *S. sanguinis* adalah bakteri yang paling banyak dalam biofilm rongga mulut dan berkorelasi dengan kesehatan mulut, terutama karies gigi dan penyakit periodontal. Penghambatan biofilm dapat dijadikan tindakan yang diperlukan untuk mengontrol biofilm. Salah satu cara adalah mengganggu dinding sel bakteri dengan menghambat biosintesis peptidoglikan. Enzim *Muramidase A* (*Mur A*) berkontribusi pada biosintesis peptidoglikan. Penelitian bertujuan untuk menganalisis aktivitas geraniol daun kemangi (*Ocimum americanum*) dengan target protein enzim *Muramidase A* dan *Glycosyltransferase P Streptococcus Sanguinis in Silico* untuk menemukan senyawa aktif yang diharapkan dapat berperan dalam eksplorasi obat.

Penelitian menggunakan metode simulasi *docking* yang memprediksi interaksi antar molekul, dapat berupa protein termasuk enzim. Struktur kristal *Muramidase A* (bank data protein ID: 1UAE) dan *Glycosyltransferase P* (bank data protein ID: 5V4a) diperoleh dari *Research Collaboratory for Structural Bioinformatics* (RCSB).

Analisis *in silico* menunjukkan geraniol sebagai penghambat enzim *Muramidase A* dan *Glycosyltransferase P*. Afinitas pengikatan terhadap enzim *Muramidase A* dan *Glycosyltransferase P* adalah -5,2 Kcal/mol dan -8,6 Kcal/mol lebih tinggi daripada klorheksidin. Hasil penelitian menunjukkan geraniol memiliki aktivitas geraniol terhadap enzim *Muramidase A* dan *Glycosyltransferase P S. sanguinis* dilihat dari *binding affinity*, jenis ikatan dan panjang ikatan secara *in silico*.

Simpulan dalam penelitian ini adalah senyawa geraniol memiliki potensi sebagai agen antibakteri alami baru melalui penghambatan enzim *Muramidase A* dan *Glycosyltransferase P Streptococcus sanguinis*.

**Kata kunci :** senyawa geraniol, *Ocimum americanum*, enzim *Muramidase A*, enzim *Glycosyltransferase P*, *Streptococcus sanguinis*, *In Silico*

## **Antibacterial Activity of the Basil Leaves' Geraniol Compound (*Ocimum Americanum*) Against the Enzyme Muramidase A and Glycosyltransferase P *Streptococcus Sanguinis* Through *In Silico***

### **ABSTRACT**

*Basil leaves Ocimum americanum has been shown to have antibacterial ability against Gram positive and negative bacteria. The largest content of O. americanum is trepenoid. Geraniol compounds, which are derivatives of terpenoids, have a percentage of 37,70 %. The natural ingredient of basil (O. americanum) is expected to be an alternative mouthwash that has an antibacterial effect on Streptococcus sanguinis biofilms. S. sanguinis is the most abundant bacteria in oral biofilms and whose presence is correlated with oral health, particularly dental caries and periodontal disease. Inhibition of biofilms can be used as a necessary action to control biofilms. One way is to disrupt the bacterial cell wall by inhibiting peptidoglycan biosynthesis. Muramidase A (Mur A) enzyme contributes to the biosynthesis of peptidoglycan. The study aimed to analyze activity of geraniol Ocimum americanum targeting enzyme protein, MurA and Glycosyltransferase P S.Sanguinis In Silico, to find active compounds that are expected to play a role in drug exploration.*

*The research was carried out by docking that predicts interactions between molecules, which can be in the form of proteins including enzymes. The crystalline structures of Muramidase A (protein databank ID: 1UAE) and Glycosyltransferase P (protein data bank ID: 5V4a) were obtained from the Research Collaboratory for Structural Bioinformatics (RCSB).*

*In silico analysis showed that geraniol was an inhibitor of the Muramidase A and Glycosyltransferase P enzymes. The binding affinity for Muramidase A and Glycosyltransferase P enzymes was  $-5.2$  Kcal/mol and  $-8.6$  Kcal/mol, higher than chlorhexidine. The results showed that the mineral compounds in basil (*O. americanum*) had antibacterial activity against the enzymes muramidase A and Glycosyltransferase P *S. sanguinis* seen from their binding affinity, type of bond and bond length in silico.*

*The conclusion in this study is that geraniol compound have potential as a new natural antibacterial agent through inhibition of Muramidase A and Glycosyltransferase P *Streptococcus Sanguinis* enzymes.*

**Key words :** *geraniol compound, Ocimum americanum, Muramidase A and Glycosyltransferase P enzymes. Streptococcus sanguinis, in silico*