ABSTRAK

Pendahuluan: Pengembangan turunan tiourea sebagai agen antibakteri menjadi area penelitian yang menarik. Turunan tiourea dapat menghambat enzim DNA gyrase b, yang merupakan enzim penting dalam replikasi DNA pada bakteri.

Tujuan: Mengetahui % *yield* serta kemurnian dan konfirmasi struktur senyawa hasil sintesis 4CC2P, mengetahui mekanisme kerja dan interaksi senyawa 4CC2P terhadap target protein secara *in silico*, dan mengetahui aktivitas antibakteri senyawa 4CC2P terhadap bakteri S. *aureus* secara *in vitro*.

Metode: Sintesis senyawa 4CC2P melalui dua tahap reaksi, yaitu reaksi S_N2 dan adisi nukleofilik. Uji kemurnian dilakukan dengan titik lebur dan KLT sedangkan konfirmasi struktur dengan spektrofotometri Uv-Vis, spektrometri IR, MS, dan ^{1}H-NMR. Uji *in silico* dilakukan dengan *docking* terhadap enzim DNA gyrase b dan *in vitro* dengan cakram difusi terhadap bakteri S. *aureus*.

Hasil: Senyawa hasil sintesis 4CC2P memiliki %yield sebesar 9,9855 %, murni, dan konfirmasi struktur mengkonfirmasi bahwa senyawa hasil sintesis benar 4CC2P. Senyawa 4CC2P memiliki skor *docking* sebesar -84,0759 ± 0,0449, lebih rendah dari pada skor *docking* amoksisilin (-82,6138 ± 0,0652). Senyawa 4CC2P memiliki aktivitas antibakteri terhadap bakteri S. *aureus* pada 2000 ppm sebesar 9,05±0,944 mm, relatif kecil dibandingkan kontrol amoksisilin pada 15 ppm sebesar 16,275±0,325 mm.

Kata Kunci : turunan tiourea, antibakteri, sintesis, *docking*, cakram difusi.

ABSTRACT

Background: The development of thiourea derivates as antibacterial has become an interesting area of research. Thiourea derivates can inhibit the DNA gyrase b enzyme, which is an important enzyme involved in bacterial DNA replication.

Aim: To determine the % yield, purity, and confirm the structure of the synthesized compound 4CC2P, to investigate the mechanism of action and interactions of the compound 4CC2P with the target protein through in silico method, and to evaluate the antibacterial activity of the compound 4CC2P against S. aureus bacteria through in vitro method.

Methods: The compound 4CC2P was synthesized through two reaction steps, namely S_N2 and nucleophilic addition. Purity testing was conducted using melting point determination and TLC, while structural confirmation was performed using UV-Vis spectrophotometry, IR spectroscopy, MS, and ^{1}H-NMR. The antibacterial activity of the compound was assessed through in silico using docking method against the DNA gyrase B enzyme and in vitro using disk diffusion method against S. aureus bacteria.

Results: The synthesized compound 4CC2P has a yield of 9,9855%, is pure, and structural confirmation confirmed that the synthesized compound is indeed 4CC2P. The docking score of 4CC2P was -84,0759 ± 0,0449, which was lower than the docking score of amoxicillin (-82,6138 ± 0,0652). The compound 4CC2P exhibited antibacterial activity at 2000 ppm with a zone of inhibition measuring 9,05±0,944 mm, which is relatively smaller compared to the control amoxicillin at 15 ppm with a zone of inhibition measuring 16,275±0,325 against S. aureus bacteria.

Keywords: thiourea derivatives, antibacterial, synthesis, docking, disk diffusion.