SINTESIS KALKON DAN PIRAZOLINA DARI 4-HIDROKSI ASETOFENON SERTA UJI AKTIVITAS SECARA *IN VITRO* DAN *IN SILICO* SEBAGAI SENYAWA KANDIDAT ANTIBAKTERI

Olivia Wulandari Pingkan Ratag
19/445681/PA/19505

INTISARI

Sintesis, studi penambatan molekuler, dan uji aktivitas antibakteri terhadap dua variasi senyawa kalkon dan dua variasi senyawa pirazolina telah berhasil dilakukan. Variasi senyawa kalkon yang diuji yakni 1-(4-hidroksifenil)-3-fenilprop-2-en-1-on (senyawa **1a**) dan 3-(3,4-dimetoksifenil)-1-(4-hidroksifenil) prop-2-en-1-on (senyawa **1b**). Adapun variasi senyawa pirazol yang diuji yakni 4-(1,5-difenil-4,5-dihidro-1H-pirazol-3-il)fenol (senyawa **2a**) dan sintesis 4-(5-(3,4-dimetoksifenil)-1-fenil-4,5-dihidro-1H-pirazol-3il)fenol (senyawa **2b**) telah berhasil dilakukan. Penelitian ini bertujuan untuk melakukan sintesis senyawa turunan kalkon dan pirazol dari 4-hidroksi asetofenon melalui reaksi kondensasi Claisen-Schmidt, serta mengetahui aktivitasnya sebagai senyawa kandidat antibakteri.

Senyawa kalkon **1a** dan **1b** disintesis dengan mereaksikan senyawa 4'-hidroksi asetofenon dan benzaldehida pada suasana basa NaOH 30% (b/v) melalui metode pengadukan. Senyawa pirazolina **2a** dan **2b** disintesis dengan mereaksikan senyawa kalkon (**1a** dan **1b)** dan fenil hidrazin pada suasana asam dengan metode refluks. Uji aktivitas secara *in silico* dilakukan dengan menambatkan senyawa terhadap protein *gyrase* B (PDB ID: 1kzn) untuk mengetahui interaksinya dengan protein target. Uji aktivitas antibakteri dilakukan dengan metode difusi cakram terhadap bakteri *S. aureus* dan *E. coli*.

Hasil penelitian didapatkan senyawa **1a**, **1b**, **2a**, dan **2b** dengan persen hasil berturut-turut adalah 98,21%; 47,48%; 23,47%; dan 14,05%. Hasil penambatan molekuler mengindikasikan bahwa seluruh senyawa memiliki penghambatan terhadap protein *gyrase* B, yaitu senyawa **1a** dan **2b** memiliki interaksi ikatan hidrogen dengan residu asam amino aktif protein *gyrase* B pada Asn46, sedangkan senyawa **1b** dan **2a** memiliki interaksi ikatan hidrogen dengan residu asam amino aktif pada Arg136. Uji aktivitas antibakteri menunjukkan senyawa **1a**, **2a**, dan **2b** memiliki kemampuan untuk menghambat bakteri *S. aureus* dan *E. coli*, sedangkan senyawa **1b** hanya dapat menghambat bakteri *S. aureus.*

Kata kunci: Antibakteri, kalkon, penambatan molekuler, pirazolina

SYNTHESIS OF CHALCONE AND PYRAZOLINE FROM 4-HYDROXY ACETOPHENONE WITH *IN VITRO* AND *IN SILICO* ACTIVITY TEST AS ANTIBACTERIAL CANDIDATE COMPOUNDS

Olivia Wulandari Pingkan Ratag
19/445681/PA/19505

ABSTRACT

Synthesis, molecular docking studies, and antibacterial activity tests on two variations of chalcone compounds and two variations of pyrazoline compounds have been successfully carried out. The variations of chalcone compounds tested were 1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-on (compound **1a**) and 3-(3,4-dimethoxyphenyl)-1-(4-hydroxyphenyl) prop-2 -en-1-on (compound **1b**). The variations of pyrazoline compounds tested were 4-(1,5-diphenyl-4,5-dihydro-1H-pyrazol-3-yl)phenol (compound **2a**) and 4-(5-(3,4-dimethoxyphenyl)-1-phenyl-4,5-dihydro-1H-pyrazol-3yl)phenol (compound **2b**). The research aimed to synthesize chalcone and pyrazoline derivative compounds from 4-hydroxy acetophenone via an aldol condensation reaction and determine their activity as antibacterial candidate compounds.

Chalcones **1a** and **1b** were synthesized by reacting 4'-hydroxy acetophenone and benzaldehyde in the alkaline of 30% (w/v) NaOH using a conventional method. Pyrazoline **2a** and **2b** were synthesized by reacting chalcone **1a** and **1b** with phenyl hydrazine under acidic conditions using the reflux method. Then, all compounds were docked against the *gyrase* B protein (PDB ID: 1kzn) to observe their interaction with the target protein. The antibacterial activity test was carried out using the disc diffusion method against *S. aureus* and *E. coli* bacteria.

These experiments had formed **1a**, **1b**, **2a**, and **2b** compounds with percent yields of 44.64%, 49.29%, 23.47%, and 14.17%, respectively. The results of molecular docking indicated that all of the compounds have *gyrase* B protein inhibition, in which **1a** and **2b** compounds form hydrogen bond interactions with active amino acid residue of protein *gyrase* B on Asn 46, whereas **1b** and **2a** compounds form hydrogen bond interactions with active amino acid residue on Arg136. The antibacterial activity test showed that **1a**, **2a**, and **2b** compounds could inhibit both *S. aureus* and *E. coli* bacteria, while **1b** compound could only inhibit *S. aureus* bacteria.

Keywords: Antibacterial, chalcone, molecular docking, pyrazoline