SENYAWA TURUNAN AZINA SIMETRIS SEBAGAI ANTIBAKTERI: PENAMBATAN MOLEKULER, SINTESIS, DAN UJI AKTIVITAS

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INTISARI

Telah dilakukan penelitian senyawa turunan azina sebagai antibakteri *E. coli* dan *S. aureus*. Penelitian meliputi penambatan molekuler, sintesis turunan azina dan uji aktivitas antibakterinya. Penelitian dilakukan dengan optimasi geometri terhadap ligan senyawa turunan azina, kemudian dilakukan penambatan molekuler. Hasil penambatan yang memiliki aktivitas terbaik dilakukan sintesis senyawa turunan azina. Elusidasi senyawa yang telah disintesis dilakukan dengan bantuan instrumen FT-IR, GC-MS, dan LC-MS. Produk hasil sintesis selanjutnya dilakukan pengujian antibakteri terhadap bakteri *E. coli* dan *S. aureus* menggunakan metode difusi cakram. Aktivitas antibakteri ditenentukan dari hasil diameter inhibisinya.

Hasil penambatan molekuler senyawa nitrovanilinazina, vanilinazina, veratraldehidazina, dan salisilaldehidazina menunjukkan interaksi ikatan hidrogen pada DNA girase dengan asam amino residu spesifik Asn46, Asp73, dan Arg136 yang memberikan energi ikatan sebesar -4,41 kJ; -4,50 kJ; -4,13 kJ; dan -4,23 kJ dengan nilai RMSD semua di bawah 2 Å. Sintesis senyawa nitrovanilinazina, vanilinazina, veratraldehidazina, dan salisilaldehidazina secara berturut-turut menghasilkan rendemen sebesar 40,96%; 48,80%; 59,63%; dan 61,04%. Uji aktivitas antibakteri menghasilkan luas penghambatan pada bakteri *E. coli* adalah 1,25 mm; 0,82 mm; 1,48 mm; dan 1,05 mm, sedangkan pada bakteri *S. aureus* didapatkan luas penghambatan adalah 2,18 mm; 1,35 mm; 1,88 mm; dan 2,15 mm. Kloramfenikol sebagai kontrol positip menghasilkan luas penghambatan pada bakteri *E. coli* dan *S. aureus* sebesar 6,75 dan 8,23 mm. Hasil semua senyawa turunan azina menunjukkan aktivitas antibakteri memiliki aktivitas lemah dibandingkan kloramfenikol.

Kata kunci: antibakteri, azina, penambatan molekuler, dan sintesis.

SYMMETRICAL AZINE DERIVATIVES AS ANTIBACTERIAL: MOLECULAR DOCKING, SYNTHESIS, AND ACITIVITY TESTING

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ABSTRACT

Research has been conducted of azine derivative compounds as antibacterial against E. coli and S. aureus. The research included molecular docking, synthesis of azine derivatives, and antibacterial activity testing. The research began with geometric optimization of the ligands of azine derivative compounds, followed by molecular docking. The azine derivative compounds showing the best activity were then synthesized. The elucidation of the synthesized compounds was carried out with FT-IR, GC-MS, and LC-MS instruments. Subsequently, the synthesized products were tested for antibacterial activity against *E. coli* and *S. aureus* using the disc diffusion method. The antibacterial activity was determined based on the inhibition zone diameter.

The results of molecular docking for nitrovanilinazine, vanilinazine, veratraldehydeazine, and salicylaldehydeazine compounds showed hydrogen bonding interaction with DNA gyrase involving specific amino acid residues Asn46, Asp73, and Arg136, providing binding energies of -4.41 kcal/mol, -4.50 kcal/mol, -4.13 kcal/mol, and -4.23 kcal/mol, respectively, with all RMSD values below 2 Å. The synthesis of nitrovanilinazine, vanilinazine, veratraldehydeazine, and salicylaldehydeazine compounds yielded yields of 41.67%, 48.80%, 57.48%, and 59.14% respectively. Antibacterial activity test resulted in inhibition zones of 1.25 mm, 0.82 mm, 1.48 mm, and 1.05 mm against *E. coli* and, 2.18 mm, 1.35 mm, 1.88 mmm, and 2.15 mm against *S. aureus*. Chloramphenicol as a positive control gave inhibition zones of 6.75 mm against *E. coli* and 8.23 mm against *S. aureus.* All azine derivative compounds exhibited weak antibacterial activity compared to the chloramphenicol.

Keywords: antibacterial, azine, molecular docking, and synthesis.