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Antibacterial Agents: Design and *in silico* Studies

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Abstract

The emergence of antibiotic resistance poses a severe threat to global health. β-lactams, a class of antimicrobial agents renowned for their broad-spectrum activity, favorable pharmacokinetic properties, low toxicity, oral bioavailability, and bactericidal action, have been a cornerstone of antimicrobial therapy.[1] These agents exert their antibacterial effect by inhibiting the catalytic activity of bacterial transpeptidases, also known as penicillin-binding proteins (PBPs), which are essential enzymes in the cross-linking of peptidoglycan chains during cell wall synthesis.[2] In this study, we designed a series of monocyclic β-lactams incorporating diverse substituents. These compounds were subsequently evaluated for their inhibitory potential against PBP, a crucial target in bacterial cell wall biosynthesis, using molecular docking simulations with the validated PDB structure 1MWT. Visual analysis of the docking results revealed favorable interactions between the designed compounds and the active site residues of PBP. Notably, several compounds exhibited promising binding affinities and could potentially serve as lead candidates for the development of novel antimicrobial agents to combat infectious diseases.

Key words: 2-Azetidinone, molecular docking, antibacterial, drug design.

References

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