Computational Approach to Identify Potential Inhibitory Molecule Against Bacterial Enzyme

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This study aimed to identify potential inhibitors of meso-diaminopimelate decarboxylase (LYASE), a bacterial enzyme crucial for lysine biosynthesis, using molecular docking simulations. The hypothesis for the study was that the binding of 3 Phi-Difluorophenylacetic Acid and 2,3 Dichlorophenyl Thiazole Carboxylic Acid would inhibit the enzyme's activity. The procedure involved docking these ligands to the active site of a modified LYASE protein using SwissDock in two box sizes(10,10,10 and 20,20,20), followed by statistical analyses to evaluate binding affinities. Both ligands demonstrated significant binding, with affinities lower than -5 kcal/mol in larger docking box sizes and strong correlations ($p=0.9602, p<0.0001$). Statistical results rejected the null hypothesis, supporting that ligand binding inhibits LYASE activity. These findings align with previous research showing the use of LYASE inhibition for antibacterial drug discovery. Unlike traditional screening methods, this study had a focused approach with fewer ligands, achieving comparable efficacy. Future work would research live bacterial studies to confirm computational predictions and assess resistance mechanisms. This research helps in addressing the global antibiotic resistance crisis by searching for inhibitors for a bacterial enzyme. The development of LYASE inhibitors has the potential to create novel treatments for multidrug-resistant bacterial infections, enhance healthcare resilience, and reduce treatment costs, showing the importance of molecular docking in fighting against antibiotic resistance and ensuring the effectiveness of life-saving medical procedures.

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