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Docking Studie of Biologically Active Molecules: Exploring Medical Applications

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Abstract : \This research explores the efficacy of novel pyrimidine derivatives on bacterial strains such as Escherichia coli, Staphylococcus aureus, and Myccobacterium tuberculosis, utilizing bending energy calculations. Of the 25 compounds examined, 13 displayed potent activity against all the bacterial strains under study, exhibiting bending energy measurements between -7.4 and -10.7 kcal/mol. The -7.4 kcal/mol value corresponds to the bending energy of the SA12 and SA13 compounds with the 2xct protein (Staphylococcus aureus), whereas the -10.7 kcal/molis linked with the bending energy of SA6 and SA11 compounds with the 6GAV protein (Myccobacterium tuberculosis). Further research will involve a QSAR (Quantitative Structure-Activity Relationship) study aimed at constructing a reliable model to combat the aforementioned bacterial strains and a molecular dynamics study to evaluate the stability of ligand-protein complexes.

Keywords : docking, QSAR, bending energy, e. coli
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