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Exploring Penicillin Resistance in Gonococcal Penicillin Binding Protein-2: Molecular Docking and Ligand Interaction Analysis

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Abstract : Gonococcal infections present a notable public health issue, and the major approach for treatment involves using β-lactam antibiotics that specifically target penicillin-binding protein 2 (PBP2) in Neisseria gonorrhoeae. This study examines the influence of flavonoids, namely rutin, on the structural changes of PBP2 in both penicillin-resistant (FA6140) and penicillin-susceptible (FA19) strains. The research clarifies the structural effects of particular mutations, such as inserting an aspartate residue at position 345 (Asp-345a) in the PBP2 protein. The strain FA6140, which is resistant to penicillin, shows specific changes that lead to a decrease in penicillin binding. These mutations, namely P551S and F504L, significantly impact the pace at which acylation occurs and the stability of the strain under high temperatures. Molecular docking analyses investigate the antibacterial activities of rutin and other phytocompounds, emphasizing its exceptional binding affinity and potential as an inhibitor of PBP2. Quercetin and protocatechuic acid have encouraging antibacterial effectiveness, with quercetin displaying characteristics similar to those of drugs. Molecular dynamics simulations offer a detailed comprehension of the interactions between flavonoids and PBP2, highlighting rutin's exceptional antioxidant effects and strong affinity for the substrate binding site. The study's wider ramifications pertain to the pressing requirement for antiviral treatments in the context of the ongoing COVID-19 epidemic. Flavonoids have a strong affinity for binding to PBP2, indicating their potential as inhibitors to impair cell wall formation in N. gonorrhoeae. Ultimately, this study provides extensive knowledge on the interactions between proteins and ligands, the dynamics of the structure, and the ability of flavonoids to combat penicillin-resistant N. gonorrhoeae bacteria. The verified simulation outcomes establish a basis for creating potent inhibitors and medicinal therapies to combat infectious illnesses.

Keywords : phytochemicals, penicillin-binding protein 2, gonococcal infection, ligand-protein interaction, binding energy, neisseria gonorrhoeae FA19, neisseria gonorrhoeae FA6140, flavonoids
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