

INSIGHTS INTO BACTERIAL INTERACTIONS: COMPARING FLUORINE-CONTAINING 1,2,4-TRIAZOLES TO ANTIBIOTICS USING MOLECULAR DOCKING AND MOLECULAR DYNAMICS APPROACHES

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The escalating challenge of antibiotic resistance necessitates innovative therapeutic strategies. We delve into the unexplored realm of Fluorine-containing 1,2,4-triazoles as potential antibacterial agents, focusing on interactions with *Staphylococcus aureus* and *Serratia marcescens*. Through quantitative assays and *in silico* approaches, we elucidate molecular docking and molecular dynamics results. Tested compounds possess exceptional binding reveals non-conventional modes. Our study highlights the intricacies of ligand-protein interactions, offering insights into antibiotic resistance combat. These findings advance antimicrobial strategies and contribute to combating evolving bacterial challenges.

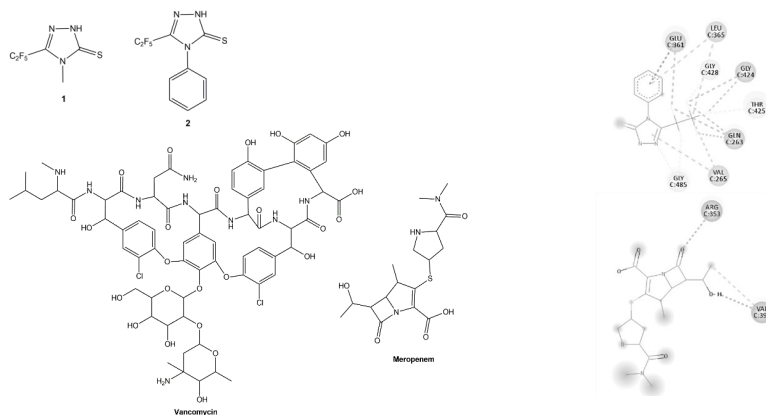


Fig. 1. Molecular formulas of investigated compounds and 2D representation of interactions between I17S with compound 2 and meropenem

In conclusion, this study's holistic approach underscores the complex landscape of antibiotic interactions with bacterial targets. The differential affinities and molecular dynamics revealed through simulations emphasize the multifaceted nature of ligand-protein interactions. The exceptional affinity of compound 1 suggests alternative binding modes, invoking a deeper exploration of non-conventional mechanisms.

These findings illuminate the potential for unconventional binding modes and further elucidate the intricate interplay of molecular attributes. As we move forward, comprehensive approaches combining simulations, structural analyses, and experimental validation will be pivotal in unraveling the mechanisms of action and guiding the development of novel antimicrobial strategies.

Ultimately, our study contributes to the broader understanding of antibiotic efficacy, providing valuable insights into the dynamic world of microbial interactions.

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