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# AI-driven virtual screening for combatting antibiotic resistance: a promising therapeutic approach

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## KEY MESSAGES

1. The compound demonstrates higher binding affinity to beta-lactamase enzymes than the commercial inhibitor clavulanic acid.
2. Molecular dynamics simulations confirm the stability of the compound under physiological conditions.
3. ADMET predictions indicate that the compound has favorable drug-likeness and pharmacokinetic properties, supporting its therapeutic potential.

## ABSTRACT

**Introduction.** The emergence of multi-resistant and pan-resistant enterobacteria to betalactam antibiotics poses a significant threat to human health. The prevailing resistance mechanism in enterobacteria involves the production of beta-lactamases, enzymes that break down the beta-lactam cycle. Thus, compounds inhibiting these enzymes seem promising candidates for potential drugs.

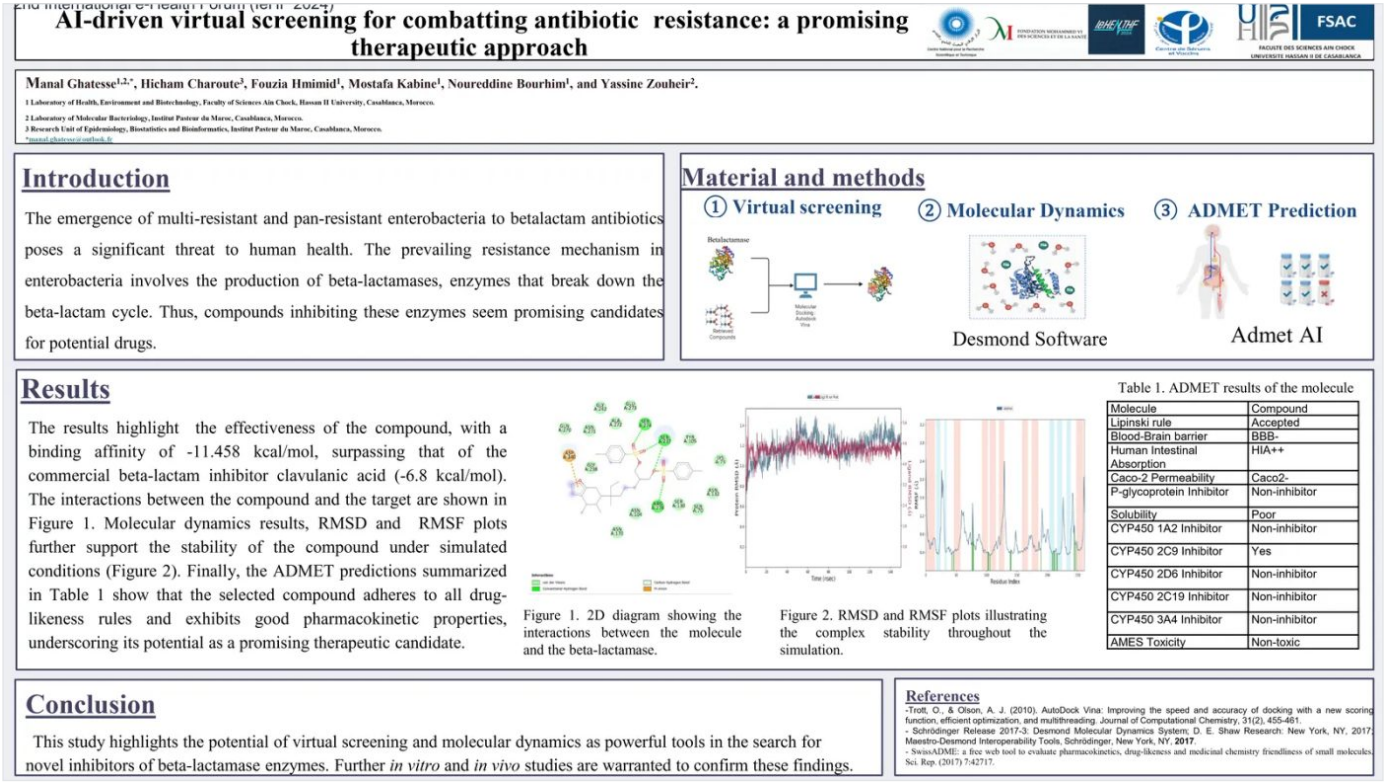
**Materials and methods.** The study employed three main methods: 1) Virtual screening using molecular docking with Autodock Vina to identify potential inhibitors of beta-lactamase enzymes; 2) Molecular dynamics simulations using Desmond software to assess the stability of the compound-target interactions; 3) ADMET prediction using Admet AI to evaluate the pharmacokinetic properties and drug-likeness of the selected compound.

**Results.** The results highlight compound's effectiveness, with a binding affinity of -11.458 kcal/mol, surpassing that of the commercial beta-lactam inhibitor clavulanic acid (-6.8 kcal/mol). Molecular dynamics results, including RMSD and RMSF plots, support the stability of the compound under simulated conditions. ADMET predictions show that the compound meets all drug-likeness rules and has good pharmacokinetic properties, underscoring its potential as a promising therapeutic candidate.

**Conclusion.** This study highlights the potential of virtual screening and molecular dynamics as powerful tools in the search for novel inhibitors of beta-lactamase enzyme. Further in vitro and in vivo studies are warranted to confirm these findings.

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