

PROTEIN-LIGAND DOCKING AND IN VITRO SCREENING AS A TOOL TO IDENTIFY LEAD HIT DRUGS TARGETING THE KEY SURVIVAL PURINE NUCLEOSIDE PHOSPHORYLASE (PNP) ENZYME OF HELICOBACTER PYLORI

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Poster

Stomach & H. Pylori

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Computer-aided drug design targeting the purine nucleoside phosphorylase enzyme identified seven compounds with antimicrobial activity against *Helicobacter pylori*, including clarithromycin-resistant strains.

KEY POINTS

- Protein-ligand docking screened over 550,000 compounds against the purine nucleoside phosphorylase enzyme, a key survival enzyme of *H. pylori*.
- All seven lead compounds tested showed antimicrobial activity against reference strains and clinical isolates of *H. pylori*, including both clarithromycin-sensitive and clarithromycin-resistant strains, with MIC50 values ranging from 4.34 to 73 µg/mL.
- Two compounds demonstrated significant selectivity, showing antimicrobial activity against *H. pylori* without affecting the viability of human gastric epithelial cells.
- The authors conclude that protein-ligand docking provided a cost-efficient method to identify selective antimicrobial agents, with several lead targets identified for further development to increase selectivity and potency.

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