
Contribution ID: **164** Type: **Poster**

# In Silico Strategy for the Identification of Novel Efflux Pump Inhibitors Targeting MexB

The escalating crisis of antimicrobial resistance (AMR) in Gram-negative bacteria, particularly Pseudomonas aeruginosa, necessitated novel treatment strategies. Efflux pump inhibitors (EPIs) emerged as a promising approach to enhance the efficacy of existing antibiotics. This report outlines a detailed computational strategy developed to identify new EPIs specifically targeting the MexB protein, a crucial component of the MexB-OprM efflux pumpThe method employed structure-based virtual screening using the co-crystallized, inhibitor-bound crystal structure of MexB (PDB ID: 3w9i). During docking with a test drug molecule, the known EPI Phenylalanine-arginyl β-naphthylamide (PAβN) was used as a benchmark, showing a binding energy of approximately −6.27 kcal/mol. For comparison, Dodecyl-β-D-maltoside exhibited a binding energy of −4.62 kcal/mol.. These results aim to guide future research, establishing a clear pathway from in silico prediction to experimental validation. This strategy has the potential to facilitate the development of clinically valuable compounds to combat multidrug resistance.

Keywords:, Efflux pump inhibitors (EPIs), MexB , Molecular docking, Virtual screening.

**Authors:** Ms P R, Akshaya (JAIN (Deemed-to-be University) School of Sciences); Dr UMAKANTH NAIK, Vankadoth (JAIN (Deemed-to-be University) School of Sciences)

**Co-author:** Mr M, Thejas (JAIN (Deemed-to-be University) School of Sciences)

**Presenter:** Ms P R, Akshaya (JAIN (Deemed-to-be University) School of Sciences)

**Track Classification:** Biological Sciences