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## COMPUTATIONAL IDENTIFICATION OF NOVEL INHIBITORS AGAINST *KLEBSIELLA PNEUMONIAE* DNA ADENINE METHYLTRANSFERASE

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*Klebsiella pneumoniae* a gram-negative bacteria causing pneumonia, urinary tract infection and liver abscess infections in the nosocomial settings. These bacterial pathogens are classified under the urgent hazard level leading towards a concern in public health. The epidemiology remains enigmatic and the current antibiotics failing to combat the emerging antimicrobial resistant bacteria. DNA methylation is seen to play a vital role in regulating the gene expression, directed mismatched repair and are seen to influence the bacterial pathogenicity. Current antibiotic-resistant studies have been progressively associated with DNA adenine methyltransferase (DAM) inhibitors, which play a crucial role in bacterial pathogenesis. Author's aim of the study is to screen novel natural inhibitor for *Klebsiella pneumoniae* DNA adenine methyltransferase. They had performed fingerprint similarity search based on Mahanine which resulted in 22 similar structures. Based on virtual screening using Autodock and ADMET test, they identified Koenimbine having a high affinity towards our previously identified protein target (A0A2U0NNR3) with -5.67kcal/mol and does not violates the Lipinski Rule of 5. This study will provide insight towards the identification of the new natural bioactive compound as a potential drug target to combat antimicrobial resistant pathogens.

## BIOGRAPHY

Umairah Natasya Mohd Omeershffudin is an undergraduate student from Management and Science University, Malaysia. Currently she is doing her final year Bachelor in Bioinformatics (Hons). Her research focusing on finding novel drug target for antimicrobial resistant bacterial pathogens using computational aided drug design.

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