Abstract No: 150 ***AI in Biomedical Sciences***

DRUG REPURPOSING FOR STREPTOCOCCUS TOXIC SHOCK SYNDROME (STSS), THE "FLESH-EATING BACTERIA" SPREADING IN JAPAN

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Streptococcus Toxic Shock Syndrome (STSS), caused by invasive group A *Streptococcus* bacteria, presents significant health challenges in Japan due to limited treatment options and increasing antibiotic resistance. This study addressed these challenges by exploring drug repurposing through a computational screening method. Using the KNIME Analytics Platform, a Machine learning pipeline screened 3000 drug candidates (primarily phytochemicals sourced from medicinal plants) against STSS using training data from 36 antibiotics. Training data were selected from current treatment practices in hospitals, while test data were chosen based on literature on antimicrobial properties. A training-validation split of 80:20 was employed, where 80% of the data was used for model training and 20% for validation to assess model performance and generalizability. The pipeline includes Random Forest (RF), Artificial Neural Network (ANN), and Support Vector Machine (SVM) models, achieving prediction accuracies of 99.84%, 99.31%, and 98.31% respectively, with corresponding Root Mean Squared Error (RMSE) values of 0.04, 0.08 and 0.13. Model performances were evaluated using precision, recall, F1 score, and Cohen's kappa metrics. From the screening, seven compounds emerged as promising candidates after validation through Pan-assay: Fosbretabulin disodium, Amphotericin B, Cysteamine, Taxol A, Tilarginine, Ascaridole, and D-Penicillamine. Ascaridole, with its natural origin and historical medicinal use, stands out for its antimicrobial and anti-inflammatory properties as a phytochemical. While further pre-clinical and clinical studies are necessary to evaluate their efficacy and safety for STSS treatment, this research used Machine learning to identify new therapeutic options for STSS through drug repurposing.

Keywords: Antibiotic resistance, Drug repurposing, KNIME, Machine learning, STSS