Elucidating RSV-Host Protein-Protein Interactions: Novel implementation of Graph Attention Networks (GAT) and Structural Visualization

Lakshminarasimhan, Aditya (School: BASIS Scottsdale)

Respiratory Syncytial Virus (RSV) poses significant health risks, especially to infants under six months and adults over 65. The objective of this study is to deepen the understanding of structural reasons behind the annual RSV's resurgence and its capability to evade immune responses. The novel solution employs a Graph Attention Network (GAT), end-to-end pipeline to elucidate RSV F-Fusion Protein-Host Interactions with Structural Visualizations. This innovative approach involves processing 136 RSV genomic strands, identifying affected peptides, and employing a multimodel-GAT trained on Protein-Protein Interactions (PPI) for interactions between the RSV Fusion proteins and ICAM-1 host protein. Remarkably, this model trained on 5600 viral and functional proteins, achieving 97% training accuracy and operates on Google Colab, making it accessible for research and clinical applications. The approach uses genomic sequence translations, 3D predictions with AlphaFold, predicts RSV Protein-to-Host Cell interaction probabilities using Graph Attention Network, spotlights peptides resistant to mutations across different RSV strains, and delves into the specific residues' roles in protein conformation, to offer an interaction probability metric to advance molecular understanding. In conclusion, the study reveals that Domain II of the RSV F Fusion protein is the most stable segment, incurring the least mutations (only two), earmarking it as an ideal candidate for neutralizing antibodies. In contrast, Domains III, IV, and I displayed progressively more mutations—8, 36, and 60 respectively—underscoring their fluctuating stability. The solution provides critical insights for RSV intervention strategies, illustrating the impact of sophisticated computational models in medical research.

Awards Won:

Second Award of $2,000

University of Arizona: Renewal Tuition Scholarship

The University of Texas at Dallas: Scholarship awards of $5,000 per year, renewable for up to four years