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In Silico Study of Transmembrane Topology of Predicted Epitopes of DENV Using Bioinformatics Tools

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Structured Abstract

Background: Dengue virus (DENV) remains a major global health concern due to its widespread prevalence and significant disease burden, particularly in tropical and subtropical regions. Despite extensive research, the genetic variability of the virus and the interplay between its serotypes complicate the development of effective therapeutics. Furthermore, understanding its transmembrane topology and immune evasion mechanisms is critical for advancing vaccine design. This research is significant in predicting the 3D structure of DENV membrane proteins through *in silico* analysis, demonstrating that bioinformatics can accelerate the identification of DENV epitopes.

Methods: This study aimed to predict the topological membrane structure of DENV using bioinformatics tools, visualize the 3D structure of its predicted epitopes, and compare the predicted epitopes using I-TASSER and SWISS-MODEL. Two B-cell epitope sequences, EP12 and EP15, were obtained from a previous study. The models were validated using Ramachandran analysis to assess stereochemical quality of predicted structures. MolProbity was employed to evaluate the backbone dihedral angles and side-chain conformations. SWISS MODEL validation metrics, including GMQE and QMEAN were used to further confirm model reliability and structural integrity.

Results: I-TASSER demonstrated EP12 had better model quality with a higher C-score (0.27) compared to EP15 (-0.53), within the cutoff value of -5 to 2. Similarly, SWISS-MODEL highlighted the structural robustness of EP12 with a higher GMQE (0.76) compared to EP15 (0.54), adhering to the cutoff value of 0.4 to 1.0 (Bienert et al., 2016). Visualization revealed that β-sheet dominance in EP12 contributed to greater structural stability and consistent immune targeting, while loop-dominated structure in EP15 resulted in higher flexibility but less rigidity. Validation further confirmed the robustness of EP12, with 94.12% favoured residues and no outliers in Ramachandran analysis, compared to EP15 (64.71%). These results highlight EP12's structural stability and immune-targeting potential, while EP15's flexibility may offer alternative avenues for future enhancements.

Conclusion: These findings underscore EP12's potential as a vaccine candidate and demonstrate the effectiveness of bioinformatics tools in structural predictions. While EP12 exhibited superior structural stability, EP15's loop-dominated structure suggests potential for further study to improve flexibility and design novel immune-targeting strategies.

Keywords: Dengue virus, epitope prediction, bioinformatics, I-TASSER, SWISS-MODEL

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