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EXPLORING SAND FLY SALIVARY PROTEINS TO DESIGN MULTI-EPITOPE BASED SUBUNIT VACCINE TO FIGHT AGAINST VISCERAL LEISHMANIASIS

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Background: Visceral leishmaniasis (VL) is a serious public health issue which causes >30,000 death/year in 70 countries. Here, we have explored sandfly salivary proteins and followed comprehensive immunoinformatics approach to design multi-epitope subunit vaccine which may elucidate humoral, cell mediated and innate immune responses.

Methodology: Sandfly salivary proteins were employed for prediction of B cell and T cell binding epitopes. TLR4 agonist 50S ribosomal L7/L12 (Locus RL7_MYCTU) was chosen as adjuvant at the N-terminal followed by CTL and HTL epitopes. This vaccine construct was studied for investigating B cell binding and IFN-γ inducing epitopes. This was followed by prediction of antigenicity, allergic nature and physiochemical properties of the vaccine construct after which generation, refinement and validation of the vaccine model were performed. The interactions of this vaccine model with its immune receptor were explored by performing molecular docking and molecular dynamics simulation. Further, efficiency of expression of this vaccine construct in an expression vector, in silico cloning was performed at the final stage of vaccine design.

Result: The multi-epitope subunit vaccine construct consist of 8 CTL and 15 HTL epitopes. Final 903 amino acids vaccine constructs have shown B cell epitopes (humoral response) and INF-γ epitopes (cell mediated immune response). Vaccine construct was found to be non-allergen, antigenic and valid 3D protein structure was confirmed by Ramachandran plot. Molecular docking and dynamics simulation experiments have shown significant interaction with the TLR4 receptor present on the surface of immune cells. Wrangler and gene synthesis wizard and GeneScript rare codon analysis have shown good expression of vaccine construct in E. coli.

Conclusion: Applied comprehensive immunoinformatics approaches have designed a multi-epitope subunit vaccine, which necessitates experimental and clinical investigation to develop as an immunogenic vaccine candidate to prevent VL infection.

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