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A Study on the Prediction of Epitope-based Vaccine Candidate with Higher Efficacy for Tetanus Using Immunoinformatic Methods

Pinto MKH¹, Manaram AGI¹, Gayantha RDG¹, Madhumadhawa DMA¹, Sumanathilaka WKD¹, Herath HMRDS¹, Ranadeva NDK¹, Pathirana S²

¹Department of Biomedical Science, Faculty of Health Sciences, KIU, Battaramulla, Sri Lanka

²Research Institute for Farm Animal Biology (FBN), 18196 Dummerstorf, Germany

Background: Tetanus is an acute, life-threatening disease caused by the neurotoxin of *Clostridium tetani*. Despite existing vaccines, it remains a global health concern due to limitations such as adverse effects and the need for repeated boosters. With precision medicine advancing, epitope-based vaccines represent the next generation of safer, more stable, and targeted immunization. This study applied immunoinformatic methods to identify potential epitope-based vaccine candidates against tetanus toxoid.

Objective: To predict the epitope-based vaccine candidates with higher efficacy for tetanus using immunoinformatic methods.

Methods: The tetanus toxin protein sequence (P04958), comprising 1315 amino acids, was retrieved from the UniProt database. B-cell and T-cell epitopes were predicted using IEDB analysis tools. Epitopes were screened for antigenicity, allergenicity, toxicity and solubility. Selected epitopes were evaluated for HLA binding affinity using IEDB MHC binding tool and conservancy among homologous proteins to further scrutinize the finalized epitopes. The top shortlisted epitopes were structurally modelled using Swiss-Model and PSIPRED. The predicted protein construct was further validated by molecular docking with TLR and *in silico* cloning to simulate its expression in host systems.

Results: The final vaccine construct consisted with 19 B-cell and 19 T-cell epitopes with higher antigenicity and solubility and without allergenicity or toxicity. These predicted epitopes showed higher conservancy among selected homologous proteins with 100% identity. Further, these epitopes were high-affinity binders to selected HLA alleles with IC₅₀ < 50 nM. Protein docking revealed strong interactions with their receptors. With TLR4, an optimal docking score of -231.23 was obtained. *In silico* cloning confirmed the construct's expression potential in host systems.

Conclusion: These findings suggest that the identified epitopes hold strong immunogenic potential for developing safer, targeted epitope-based tetanus vaccines than traditional vaccines. The study supports the application of *in silico* tools in vaccine design, warranting further experimental validation.

Keywords: Epitope-based vaccine, Immunoinformatic methods, Tetanus