

Title of work: Multi-Epitope Vaccine Design against Monkeypox Virus via Reverse Vaccinology Method Exploiting Immunoinformatic and Bioinformatic Approaches

Summary:

This work focuses on the development of a multiepitope vaccine for monkeypox virus (MPXV) using immunoinformatics strategies. MPXV is a concerning pathogen with limited preventive measures available, and existing vaccines offer only moderate protection, especially in certain populations. Therefore, innovative treatment approaches are needed.

The study utilizes reverse vaccinology, genetic, and proteomic data to design an epitope-based vaccine. Epitope-based vaccines have shown promising results in terms of safety, efficacy, and feasibility. The authors aim to generate immunogenic responses in individuals infected with MPXV.

The vaccine design involves selecting B-cell epitopes, MHC-I epitopes, and MHC-II epitopes, which are connected using linkers and adjuvant peptide sequences. Various bioinformatics tools are employed to assess the antigenicity, physicochemical properties, and stability of the vaccine construct. The predicted 3D structure is refined, and its ability to bind to the TLR2 immune cell receptor is evaluated through molecular docking studies.

Molecular dynamics simulations confirm the stability of the docked complex. The recombinant vaccine protein is expressed in *Escherichia coli* using codon optimization. Immunological simulations demonstrate an increase in immune responses, including the generation of memory B-cells, T-cells, and helper T-cells.

While the results are promising, further in vitro and in vivo research is required to evaluate the vaccine's efficacy against MPXV. The designed protein sequence can be synthesized for expression studies, followed by preclinical and clinical investigations.

In conclusion, this work presents a novel approach for developing a multiepitope vaccine for MPXV using immunoinformatics. The study highlights the potential of epitope-based vaccines and lays the foundation for future research in combating MPXV.



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