





Vaccine Design for MPXV

DHANYASHRI A/P GURUPARAN 012022020020



FINAL PROJECT PRESENTATION 22/12/2022





Introduction

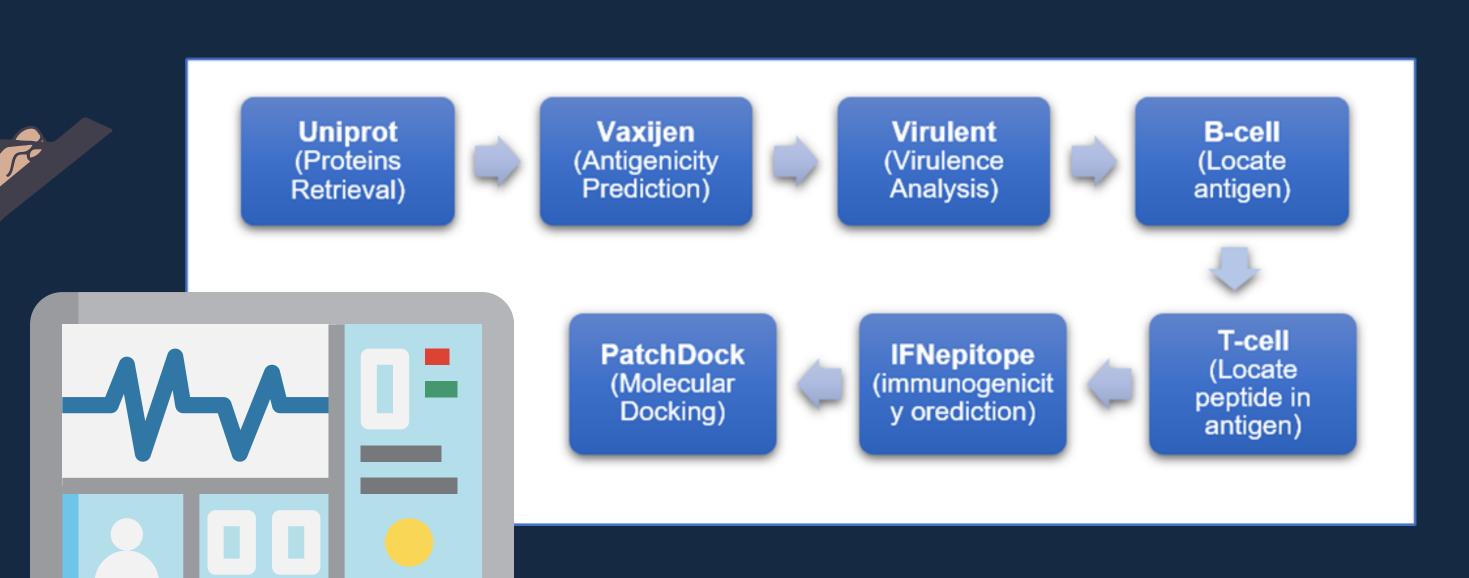
- Monkeypox is an uncommon zoonotic disease isolated to West and Central African forests in the twentieth century
- The epidemic of human monkeypox in various nations since May 2022 has been exceptional in terms of the high number of cases
- There is no conventional MPV vaccination available
- **04** Vaccinating individuals against MPXV is currently a critical necessity.







Materials & Methods





Results & Discussions







MPXV Sequence	Antigen Score	Antigen/Non- Antigen	Results
MPXV A33R	0.4775	Antigen	Vession EDILLES Model selected: virus Theredold for this model: 8.4 Non Vegenore N
MPXV H3L	0.4684	Antigen	Model selected: virus Tarchold for this model is a See Taylor of the selected of the selecte
MPXV M1R	0.6173	Antigen	Threshold for this model: 0.4 Near Sequence: ###################################
MPXV L1R	0.4085	Antigen	Vacadous SCINCLES Model selected: virus Threshold for this model: 0.4 Vant Sequence: PERSONAL SECURITY SECU

Table 1.0: Vaxijen prediction results of 4 different monkeypox sequence analyses

conserved portions reveals that all of the antigenic regions satisfied VaxiJen's standard criteria of 0.4.

MPXV Sequence	Virulent Result	Virulent Score	Results				
MPXV A33R	Virulent	1.0645	No. Profess Notes Profess results Profess Serve				
MPXV H3L	Virulent	0.4979	5. No. Protois Name Professe results Producted Scenes Concade of SVNds and PNI- BLAST -68FXV BULQUECT2QCCC2_MONRY 2nfv In partic hading surface protois ON-Nikolangum Name ON-0004 ON-0004, PL-4 SV-1				
MPXV M1R	Virulent	0.9963	S. No. Profess Negative Production condition Production forces				
MPXV L1R	Virulent	1.0501	S.No. Protein Name Proteins month: Proteins Some				

Table 2.0: Virulent prediction results of 4 different monkeypox sequence analyses.

proteins are non-allergenic, non-toxic, and is virulent implying that host cell-induced immunogenic responses target only the virus rather than the host





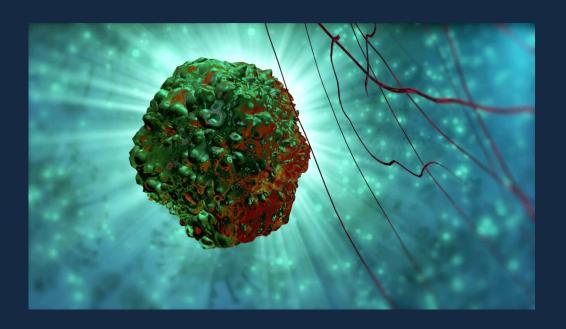


MPXV Sequence	Peptide	Length	Antigen Score	Antigen/ Non- Antigen	Results
MPXV A33R	FLEKTSFYNCN DSITKEKIKI	21	0.2106	Non- Antigen	Name and the second of the sec
	KVNNNYNNYNN YNCYNNYNCYNYDDTFF	28	0.8273	Antigen	Model selected: virus Servidal for the model to the beginner Servidal for the model to the beginner Servidal decision to the beginner of the beginner Servidal decision to the beginner of the
MPXV H3L	PPSETFPNVHEHINDQ KFDDVKDNEVMQEKRD VVIVNDDPDHY	43	0.4473	Antigen	Model referred; virus Model referred; virus Novelette de mod tot for lagrac 1 to the model tot transport of the total tota
	ALWDSKFFTELENKN	15	0.8294	Antigen	Model selected: virus Nodel selected: virus Nodel to the model to ver loyene 1 2000000 10000 Table to the boston large - 96290 Subde 1/4900410
	ITGNKVKTELVIDKDH	18	0.2125	Non- Antigen	Model selected: 1 irus Novice to select 12 Sevented to the solet 12 Sevented to the select
MPXV M1R	AALNIQTSVNTVVRDF ENYVKQTCN	25	0.2174	Non- Antigen	Model calected: Virus Model to selected: Virus Needed to the seden to I Needed to the seden to I Needed to the seden to I Needed to the seden to II Needed to the seden to III Needed to the seden to IIII to III
	KATTQIAPRQVAGT	14	0.6627	Antigen	Number south 20 Microbid sorterational in literary Texture the the south in it from trapeace south parties of the literary trapeacy of the literary trapeacy traped trades to the transmission of 46400 feeting of 46400 to
MPXV L1R	KLEAVGHCYESLSE EYRQLTKFTDSQDFKK LFNKVPIVTD	40	0.0919	Non- Antigen	Model selected: Name Model selected: Name Seatestin to seal of the selected of

Table 3.5: Summary table of filtered B-cell epitope prediction results of 4 different monkeypox sequences with lengths 14 and above.

Results & Discussions

Eight conserved peptides with a length of more than 14 amino acids were selected from the server's results to execute the antigenicity test again.







Results & Discsussion



the MHC class-I T cell epitope predictions based on the percentile rank of <= 0.05% for each MHC allele and length combination to cover most of the immune responses. Meanwhile, for MCH-II-related peptides, each peptide was correlated to the alleles it was associated with where selections were based on a consensus percentile rank of 99% and above.

IFNEpitope

The projected ability of the submitted monkeypox peptides to trigger IFN-gamma was used to rank and order them and only positive results were selected

Overlapping residues

Manual comparison and cut-off values were used to choose overlapped B-cell, T-cell, and IFN epitopes to verify that the developed vaccine might elicit both host immune and cytotoxic immunogenicity

• Docking

Ligand	Receptor	Solution Number	Global Energy	Attractive VdW	Repulsive VdW	ACE	НВ
MPXV A33R	TLR4	6	-10.65	-10.67	1.40	8.02	-1.72
MPXV H3L	TLR4	7	-7.58	-17.97	5.87	7.69	-2.08
MPXV M1R	TLR4	7	-23.79	-32.18	11.34	-1.24	-1.66

Table 3.19: Docking results of each MPXV vaccine target with TLR4 after refinement using Patchdock Webserver.

Based on its minimum global energy, MPXV M1R was chosen as the most suitable vaccine design









Results & Discsussion

a) MCH-I

Peptide	Alleles	Percentile Rank	
	HLA-A*03:01	0.01	
SLNRTIVTK	HLA-A*11:01	0.03	
	HLA-A*11:01	0.01	
VTSSGAIYK	HLA-A*03:01	0.05	
MTSILNTLR	HLA-A*68:01	0.04	
KVNNNYNNY	HLA-A*30:02	0.01	
GVTSSGAIYK	HLA-A*11:01	0.03	
RFLEKTSFY	HLA-A*30:02	0.02	
FYKPKHSTV	HLA-B*08:01	0.03	
IYHDDLVVL	HLA-A*24:02	0.05	

 Table 3.6: Table of B-cell epitope prediction results (MHC-I Binding Predictions) of MPXV

 A33R monkeypox sequence.

b) MCH-II

Allele	Method	Peptide	Percentile Rank	Adjusted Rank
HLA-DRB3*01:01	Consensus (comb.lib./smm/nn)	YNCYNYDDTFFDDDD	0.52	0.52
HLA-DRB3*01:01	Consensus (comb.lib./sppp/gg)	NYNCYNYDDTFFDDD	0.59	0.59
HLA-DRB3*01:01	Consensus (comb.lib./sppp/00)	NNYNCYNYDDTFFDD	0.76	0.78
HLA-DRB1*03:01	Consensus (sam/on/styrojola)	GKVTINDLKMMLFYM	0.86	0.88
HLA-DRB1*03:01	Consensus (amm/m/stumiolo)	KVTINDLKMMLFYMD	0.86	0.86
HLA-DRB1*03:01	Consensus (sam/on/styrojola)	LGKVTINDLKMMLFY	0.88	0.88
HLA-DRB1*03:01	Consensus (sam/an/sturniola)	VLGKVTINDLKMMLF	0.91	0.91
HLA-DRB1*03:01	Consensus (Sam/an/stunicla)	VVLGKVTINDLKMML	0.94	0.94
HLA-DRB3*01:01	Consensus (comb.lib./sppn/nn)	YNNYNCYNYDDTFFD	1.30	1.30
HLA-DRB1*15:01	Consensus (span/po/sturniolo)	KGMLFVFYKPKHSTV	1.40	1.40

Table 3.9: Table of B-cell epitope prediction (MHC-II Binding Predictions) results of MPXV A33R monkeypox sequence.

a) MPVX A33R

B-Cell Epitope	MCH-I Epitope	MCH-II Epitope	IFN Gamma Positive Score	
FLEKTSFYNCN DSITKEKIK	RFLEKTSFY	YNCYNYDDTFFDDDD	0.57338052	
KVNNNYNNYNNYN CYNNYNCY NYDDTFF	KVNNNYNNY	NNYNCYNYDDTFFDD	0.38477612	

Table 3.15: Table of epitopes with overlapping residues after **[FNepitope** prediction for MPXV A33R.

a) MPXV A33R

Epitope Name	Sequence	Method	Result	Score
Epitope1_A33R_	YNCYNYDDTFFDDDD	SVM based	Positive	0.57336052
Epitope2_A33R_	NYNCYNYDDTFFDDD	SVM based	Positive	0.36477612
Epitope3_A33R_	NNYNCYNYDDTFFDD	SVM based	Positive	0.15087603
Epitope9_A33R_	YNNYNCYNYDDTFFD	SVM based	Positive	0.34938794

Table 3.14: Table of IFNepitope prediction results of MPXV A33R monkey





Conclusion

- The MPXV M1R vaccine design was shown to have the minimum global energy and ligand binding for the TLR4 receptor in all of the analyses carried out in this paper.
- It is understood that the MPXV M1R vaccination has the capacity to elicit immune cellular and humoral reactions against the MPXV.

