

Results

1. Vaxijen Prediction

MPXV Sequence	Antigen Score	Antigen/Non-Antigen	Results
MPXV A33R	0.4775	Antigen	<p>Vaxijen RESULTS</p> <p>Model selected: virus</p> <p>Threshold for this model: 0.4</p> <p>Your Sequence:</p> <pre> MPVAGINGIN MPVMPVCFMRETFVIR SGHARFVMTSILATLFLKTSFFNCHDS ITKEKIKRSGMLFVFRKSTVYKLSG SGTVSGVFLGRVTLQMLFVRELDTW GVTSSGATLGLSSIDRLSLNRTVTVNNH INSHYNYNYNYNYNYNYNYNYNYNYNY </pre> <p>Overall Prediction for the Protective Antigen = 0.4775 (Probable ANTIGEN).</p>
MPXV H3L	0.4684	Antigen	<p>Vaxijen RESULTS</p> <p>Model selected: virus</p> <p>Threshold for this model: 0.4</p> <p>Your Sequence:</p> <pre> MPVHLGITQIT MPVIMVHEFARININDIN GSPFALPRTINMRETYTISGSHLPES MVAANTFVIVFVIDRFFSETFFVHERIN DQFTGVKNGVGEKDDVIVLDQWHTED PFTQWQGHIGQKSTHFFSGQDHTCE BTKSHIARHLAMQKFFTELEHREVEYVI DEKHWIEDITFLAPVSAKHSKILIQH EITGNKVKTELVIDKHAIFTYGGYDVL DAYIIRVTTALNIVDEINSGLSGGFFFEI KRIEMKHWQIMQNSANYDEKSLVRAH RFTNKHFWERIGTYAKRYFQWMTTTF LSEFFGLDINVLGLVILFIMHMLFNVES KLNFGTGTFTAFI </pre> <p>Overall Prediction for the Protective Antigen = 0.4684 (Probable ANTIGEN).</p>
MPXV M1R	0.6173	Antigen	<p>Vaxijen RESULTS</p> <p>Model selected: virus</p> <p>Threshold for this model: 0.4</p> <p>Your Sequence:</p> <pre> MPVMRQIQI MPVIMVMEMRANEPRTINS MREYFVIRSGMRFSQWGAASIQTTVNT LSERIISKLEGSANASQTKDIONFYIR QNRGCHITVKNMCSADADAQLDAVLSAATET YSLTTEQKAVPAMFTAALIQTSVNTVVR DFENYVQTCNSAVVNKLKIQNVIIDECY GAPSGFTMLKITVYSSGKCAIKALAQTT KATTQIAPROVAGTVQFYMIVIGVILAL PMYAKMLFTSTNRIKLLANENVRHWT INDTFFRTSMIATTDIGN </pre> <p>Overall Prediction for the Protective Antigen = 0.6173 (Probable ANTIGEN).</p>
MPXV L1R	0.4085	Antigen	<p>Vaxijen RESULTS</p> <p>Model selected: virus</p> <p>Threshold for this model: 0.4</p> <p>Your Sequence:</p> <pre> MPVLRQINQIN MPVLRGMRKEFFVIRSGN LRFESVNRHQTLLTMFACDDFFKTFASQ DQSSGGLIQTVYVQPLLLIQSHQMLE AVGHCTESLEETRLTKFTSQDFKKLFNK VPVITGQVLENGYLTDFVLSMRFFKESA LATTADFPVYIPFDOLAFVNDLSSNK VEQ </pre> <p>Overall Prediction for the Protective Antigen = 0.4085 (Probable ANTIGEN).</p>

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

2. Virulent Prediction

MPXV Sequence	Virulent Result	Virulent Score	Results												
MPXV A33R	Virulent	1.0645	<table> <tr> <th>S.No.</th><th>Protein Name</th><th>Prediction results</th><th>Predicted Scores</th></tr> <tr> <td>Cascade of SVMs and PSI-BLAST</td><td></td><td></td><td></td></tr> <tr> <td>1.</td><td>>MPXV A33R:Q5IXN2/Q5IXN2_MONPV MPXV-COP-136 OS=Monkeypox virus OX=10244 GN=A33R PE=4 SV=1</td><td>Virulent</td><td>1.0645</td></tr> </table>	S.No.	Protein Name	Prediction results	Predicted Scores	Cascade of SVMs and PSI-BLAST				1.	>MPXV A33R:Q5IXN2/Q5IXN2_MONPV MPXV-COP-136 OS=Monkeypox virus OX=10244 GN=A33R PE=4 SV=1	Virulent	1.0645
S.No.	Protein Name	Prediction results	Predicted Scores												
Cascade of SVMs and PSI-BLAST															
1.	>MPXV A33R:Q5IXN2/Q5IXN2_MONPV MPXV-COP-136 OS=Monkeypox virus OX=10244 GN=A33R PE=4 SV=1	Virulent	1.0645												
MPXV H3L	Virulent	0.4979	<table> <tr> <th>S.No.</th><th>Protein Name</th><th>Prediction results</th><th>Predicted Scores</th></tr> <tr> <td>Cascade of SVMs and PSI-BLAST</td><td></td><td></td><td></td></tr> <tr> <td>1.</td><td>>MPXV H3L:Q5IXT2/Q5IXT2_MONPV IMV heparin binding surface protein OS=Monkeypox virus OX=10244 GN=H3L PE=4 SV=1</td><td>Virulent</td><td>0.4979</td></tr> </table>	S.No.	Protein Name	Prediction results	Predicted Scores	Cascade of SVMs and PSI-BLAST				1.	>MPXV H3L:Q5IXT2/Q5IXT2_MONPV IMV heparin binding surface protein OS=Monkeypox virus OX=10244 GN=H3L PE=4 SV=1	Virulent	0.4979
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MPXV M1R	Virulent	0.9963	<table> <tr> <th>S.No.</th><th>Protein Name</th><th>Prediction results</th><th>Predicted Scores</th></tr> <tr> <td>Cascade of SVMs and PSI-BLAST</td><td></td><td></td><td></td></tr> <tr> <td>1.</td><td>>MPXV M1R:Q5IXU5/Q5IXU5_MONPV IMV membrane protein OS=Monkeypox virus OX=10244 GN=M1R PE=4 SV=1</td><td>Virulent</td><td>0.9963</td></tr> </table>	S.No.	Protein Name	Prediction results	Predicted Scores	Cascade of SVMs and PSI-BLAST				1.	>MPXV M1R:Q5IXU5/Q5IXU5_MONPV IMV membrane protein OS=Monkeypox virus OX=10244 GN=M1R PE=4 SV=1	Virulent	0.9963
S.No.	Protein Name	Prediction results	Predicted Scores												
Cascade of SVMs and PSI-BLAST															
1.	>MPXV M1R:Q5IXU5/Q5IXU5_MONPV IMV membrane protein OS=Monkeypox virus OX=10244 GN=M1R PE=4 SV=1	Virulent	0.9963												
MPXV L1R	Virulent	1.0501	<table> <tr> <th>S.No.</th><th>Protein Name</th><th>Prediction results</th><th>Predicted Scores</th></tr> <tr> <td>Cascade of SVMs and PSI-BLAST</td><td></td><td></td><td></td></tr> <tr> <td>1.</td><td>>MPXV L1R:Q3I7N2/Q3I7N2_MONPV L1R OS=Monkeypox virus OX=10244 GN=L1R PE=4 SV=1</td><td>Virulent</td><td>1.0501</td></tr> </table>	S.No.	Protein Name	Prediction results	Predicted Scores	Cascade of SVMs and PSI-BLAST				1.	>MPXV L1R:Q3I7N2/Q3I7N2_MONPV L1R OS=Monkeypox virus OX=10244 GN=L1R PE=4 SV=1	Virulent	1.0501
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Cascade of SVMs and PSI-BLAST															
1.	>MPXV L1R:Q3I7N2/Q3I7N2_MONPV L1R OS=Monkeypox virus OX=10244 GN=L1R PE=4 SV=1	Virulent	1.0501												

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

3. B-Cell Epitope Prediction

a) **ID:** MPXV A33R

Predicted peptides:

No. ⬆	Start ⬆	End ⬆	Peptide ⬆	Length ⬆
1	10	30	FLEKTSFYNCNDSITKEIKI	21
2	44	46	HST	3
3	56	56	I	1
4	101	105	RLSLN	5
5	111	138	KVNNNNYNNYNNYNNYNNYNNYDDTF	28

No	Start	End	Peptide	Length	Antigen Score	Antigen/Non-Antigen
1	10	30	FLEKTSFYNCNDSITKEKIKI	21	0.2106	Non-Antigen
2	44	46	HST	3	-	-
3	56	56	I	1	-	-
4	101	105	RLSLN	5	-	-
5	111	138	KVNNNNYNNNNYNNCYNNNNY CYNYYDDTFF	28	0.8273	Antigen

Table 3.1: B-cell epitope prediction results of MPXV A33R monkeypox sequence analyses.

b) ID: MPXV H3L

Predicted peptides:

No.	Start	End	Peptide	Length
1	17	59	PPSETFPNVHEHINDQKFDDVVDNEVMQEKRDVVIVNDOPDHY	43
2	67	78	WTGGNIRDDDKY	12
3	103	117	ALWDSKFFTELENKN	15
4	130	131	IE	2
5	157	172	ITGNKVKTELVIDKDH	16
6	204	209	KSGGLS	6
7	224	225	KI	2
8	231	232	DN	2
9	234	239	AKYVEH	6
10	248	255	RFETMKPN	8

No	Start	End	Peptide	Length	Antigen Score	Antigen/Non-Antigen
1	17	59	PPSETFPNVHEHINDQKFDDVVDNEVMQEKRDVVIVNDOPDHY	43	0.4473	Antigen
2	67	78	WTGGNIRDDDKY	12	-	-
3	103	117	ALWDSKFFTELENKN	15	0.6294	Antigen
4	130	172	IE	2	-	-
5	157	209	ITGNKVKTELVIDKDH	16	0.2125	Non-Antigen
6	204	209	KSGGLS	6	-	-
7	224	225	KI	2	-	-
8	231	232	DN	2	-	-
9	234	239	AKYVEH	6	-	-
10	248	255	RFETMKPN	8	-	-

Table 3.2: B-cell epitope prediction results of MPXV H3L monkeypox sequence analyses.

c) ID: MPXV M1R

Predicted peptides:

No.	Start	End	Peptide	Length
1	23	32	EQEANASAQT	10
2	41	48	FYIRQNHG	8
3	58	63	SADADA	6
4	79	86	LTPEQKAY	8
5	93	117	AALNIQTSVNTVVRDFENYVKQTCN	25
6	136	141	CYGAPG	6
7	169	182	KATTQIAPRQVAGT	14
8	223	227	KENVH	5

No	Start	End	Peptide	Length	Antigen Score	Antigen
1	23	32	EQEANASAQT	10	-	-
2	41	48	FYIRQNHG	8	-	-
3	58	63	SADADA	6	-	-
4	79	86	LTPEQKAY	8	-	-
5	93	117	AALNIQTSVNTVVRDFENYVKQTCN	25	0.2174	Non-Antigen
6	136	141	CYGAPG	6	-	-
7	169	182	KATTQIAPRQVAGT	14	0.6607	Antigen
8	223	227	KENVH	5	-	-

Table 3.3: B-cell epitope prediction results of MPXV M1R monkeypox sequence analyses.

d) ID: MPXV L1R

Predicted peptides:

No.	Start	End	Peptide	Length
1	23	30	ASQDDESS	8
2	54	93	KLEAVGHCHYESLSEEYRQLTKFTDSQDFKKLFNKVPIVTD	40
3	114	125	KKESALATTAID	12
4	127	137	VRYIDPRRDIA	11

No	Start	End	Peptide	Length	Antigen Score	Antigen
1	23	30	ASQDDESS	8	-	-
2	54	93	KLEAVGHCHYESLSEEYRQLTKFT DSQDFKKLFNKVPIVTD	40	0.0919	Non-Antigen
3	114	125	KKESALATTAID	12	-	-
4	127	137	VRYIDPRRDIA	11	-	-

Table 3.4: B-cell epitope prediction results of MPXV L1R monkeypox sequence analyses.

MPXV Sequence	Peptide	Length	Antigen Score	Antigen/ Non-Antigen	Results
MPXV A33R	FLEKTSFYNCN DSITKEKIKI	21	0.2106	Non-Antigen	
	KVNNNNYNNYNN YNCYNNYNCYNYDDTFF	28	0.8273	Antigen	
MPXV H3L	PPSETFPNVHEHINDQ KFDDVKDNEVMQEKR VVIVNDDPDHY	43	0.4473	Antigen	
	ALWDSKFFTELENKN	15	0.6294	Antigen	
	ITGNKVKTELVIDKDH	16	0.2125	Non-Antigen	
MPXV M1R	AALNIQTSVNTVVRDF ENYVKQTCN	25	0.2174	Non-Antigen	
	KATTQIAPRQVAGT	14	0.6627	Antigen	
MPXV L1R	KLEAVGHCHYESLSE EYRQLTKFTDSQDFKK LFNKVPIVTD	40	0.0919	Non-Antigen	

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

4. T-Cell Epitope Prediction

T-Cell Epitope for MPXV A33R

a) MCH-I

Peptide	Alleles	Percentile Rank
SLNRTIVTK	HLA-A*03:01	0.01
	HLA-A*11:01	0.03
VTSSGAIYK	HLA-A*11:01	0.01
	HLA-A*03:01	0.05
MTSILNTLR	HLA-A*68:01	0.04
KVNNNNYNNY	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
IYHDDLVL	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./simm/nn)	YNCYNYDDTFFDDDD	0.52	0.52
HLA-DRB3*01:01	Consensus (comb.lib./simm/nn)	NYNCYNYDDTFFDDD	0.59	0.59
HLA-DRB3*01:01	Consensus (comb.lib./simm/nn)	NNYNCYNYDDTFFDD	0.76	0.76
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	GKVTINDLKMMLFYM	0.86	0.86
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	KVTINDLKMMLFYMD	0.86	0.86
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	LGKVTINDLKMMLFY	0.88	0.88
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	VLGKVTINDLKMMLF	0.91	0.91
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	VVLGKVTINDLKMMML	0.94	0.94
HLA-DRB3*01:01	Consensus (comb.lib./simm/nn)	YNNYNCYNYDDTFFD	1.30	1.30
HLA-DRB1*15:01	Consensus (simm/nn/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.

T-Cell Epitope for MPXV H3L

a) MCH-I

Peptide	Allele	Percentile Rank
RYPGVMYTF	HLA-A*24:02	0.01
	HLA-A*23:01	0.01
NVIEDITFLR	HLA-A*68:01	0.01
ETMKPNFWSR	HLA-A*68:01	0.01
	HLA-A*33:01	0.01
KRYPGVMYTF	HLA-A*24:02	0.01
	HLA-A*23:01	0.01
RQIMDNSAKY	HLA-B*15:01	0.01
	HLA-B*15:01	0.04
SLSAYIIRV	HLA-A*02:03	0.01
	HLA-A*02:01	0.02
TMKPNFWSR	HLA-A*31:01	0.01
	HLA-A*33:01	0.01
TPVIVVPVI	HLA-B*51:01	0.01
ITFLRPVLK	HLA-A*11:01	0.01
	HLA-A*03:01	0.02
	HLA-A*30:01	0.02
ETFPNVHEHI	HLA-A*68:02	0.02
KYTHFFSGF	HLA-A*24:02	0.02
	HLA-A*23:01	0.03
QIMDNSAKY	HLA-A*26:01	0.02
NEMKINRQI	HLA-B*44:02	0.03
	HLA-B*44:03	0.04
ETFPNVHEH	HLA-A*26:01	0.03
TELENKNVEY	HLA-B*44:03	0.04

	HLA-B*44:02	0.05
NVIEDITFL	HLA-A*02:06	0.04
	HLA-A*68:02	0.04
HEHINDQKF	HLA-B*44:03	0.05
	HLA-B*44:02	0.05
FLRPVLKAI	HLA-A*02:03	0.05
TFTTPLISF	HLA-A*23:01	0.05
FTTPLISFF	HLA-A*26:01	0.05

Table 3.8: Table of T-cell epitope prediction results (MHC-I Binding Predictions) of MPXV H3L monkeypox sequence.

b) MCH-II

Allele	Method	Peptide	Percentile Rank	Adjusted Rank
HLA-DRB1*15:01	Consensus (smm/nn/sturniolo)	LIVILFIMFMLIFNV	0.26	0.26
HLA-DRB1*15:01	Consensus (smm/nn/sturniolo)	VILFIMFMLIFNVKS	0.29	0.29
HLA-DRB1*15:01	Consensus (smm/nn/sturniolo)	IVILFIMFMLIFNVK	0.33	0.33
HLA-DRB3*01:01	Consensus (comb.lib./smm/nn)	KTELVIDKDHAIFTY	0.34	0.34
HLA-DRB1*03:01	Consensus (smm/nn/sturniolo)	DVVIVNDDPDHYKDY	0.36	0.36
HLA-DRB1*03:01	Consensus (smm/nn/sturniolo)	NDNVIEDITFLRPVL	0.36	0.36
HLA-DRB1*03:01	Consensus (smm/nn/sturniolo)	VVIVNDDPDHYKDYV	0.36	0.36
HLA-DRB1*03:01	Consensus (smm/nn/sturniolo)	RDVVIVNDDPDHYKD	0.37	0.37
HLA-DRB1*07:01	Consensus (comb.lib./smm/nn)	LSAYIIRVTTALNIV	0.4	0.4
HLA-DRB1*03:01	Consensus (smm/nn/sturniolo)	DNVIEDITFLRPVLK	0.42	0.42

Table 3.9: Table of T-cell epitope prediction (MHC-II Binding Predictions) results of MPXV H3L monkeypox sequence.

T-Cell Epitope for MPXV M1R

a) MCH-I

Peptide	Allele	Percentile Rank
LANKENVHW	HLA-B*58:01	0.01
	HLA-B*57:01	0.01
	HLA-B*53:01	0.03
ILANKENVHW	HLA-B*57:01	0.05
	HLA-B*58:01	0.04
MYYAKRMLF	HLA-A*23:01	0.01
	HLA-A*24:02	0.01
KENVHWTTY	HLA-B*44:03	0.02
	HLA-B*44:02	0.02
ALMQLTTKA	HLA-A*30:01	0.02
	HLA-A*02:03	0.05
TTVNTLSER	HLA-A*68:01	0.01
VPAMFTAAL	HLA-B*07:02	0.04
VLSAATETY	HLA-B*15:01	0.01
TLSERISSK	HLA-A*03:01	0.03
AQLDAVLSA	HLA-A*02:06	0.04
QTSVNTVVR	HLA-A*68:01	0.09
APRQVAGTGV	HLA-B*07:02	0.05
KIKLILANK	HLA-A*03:01	0.04
TTYMDTFFR	HLA-A*68:01	0.02
RQVAGTGVQF	HLA-B*15:01	0.01

Table 3.10: Table of T-cell epitope prediction results (MHC-I Binding Predictions) of MPXV M1R monkeypox sequence.

b) MCH-II

Allele	Method	Peptide	Percentile Rank	Adjusted Rank
HLA-DRB3*02:02	NetMHCIIpan	TYMDTFFRTSPMIIA	1.10	1.10
HLA-DRB3*02:02	NetMHCIIpan	TFFRTSPMIIATTDI	1.20	1.20
HLA-DRB3*02:02	NetMHCIIpan	NFYIRQNHGCNITVK	1.30	1.30
HLA-DRB4*01:01	Consensus (comb.lib./smm/nn)	AVVDNKLKIQNVIID	1.40	1.40
HLA-DRB1*15:01	Consensus (comb.lib./smm/nn)	LAALFMYYAKRMLFT	1.40	1.40
HLA-DRB4*01:01	Consensus (comb.lib./smm/nn)	VVDNKLKIQNVIIIDE	1.40	1.40
HLA-DRB3*02:02	NetMHCIIpan	FYIRQNHGCNITVKN	1.50	1.50
HLA-DRB3*02:02	NetMHCIIpan	GNFYIRQNHGCNITV	1.50	1.50
HLA-DRB1*15:01	Consensus (comb.lib./smm/nn)	ILAALFMYYAKRMLF	1.50	1.50
HLA-DRB1*15:01	Consensus (comb.lib./smm/nn)	AALFMYYAKRMLFTS	1.70	1.70

Table 3.11: Table of T-cell epitope prediction (MHC-II Binding Predictions) results of MPXV M1R monkeypox sequence.

T-Cell Epitope for MPXV L1R

a) MCH-I

Peptide	Allele	Percentile Rank
YLFDFVISL	HLA-A*02:01	0.01
	HLA-A*02:06	
	HLA-A*02:03	
EEYRQLTKF	HLA-B*44:03	0.01
	HLA-B*44:02	
KLFNKPVIV	HLA-A*02:01	0.01
	HLA-A*02:06	
	HLA-A*02:03	
QYLDFLLLL	HLA-A*23:01	0.02
	HLA-A*24:02	0.03
TAIDPVRYI	HLA-B*51:01	0.04
	HLA-A*68:02	0.05
FADDDSFVKY	HLA-A*01:01	0.01
LSDILQITQY	HLA-A*01:01	0.01
NVMDILKSNK	HLA-A*68:01	0.1
SLSEEYRQL	HLA-A*02:03	0.05

Table 3.12: Table of T-cell epitope prediction results (MHC-I Binding Predictions) of MPXV L1R monkeypox sequence.

b) MCH-II

Allele	Method	Peptide	Percentile Rank	Adjusted Rank
HLA-DRB3*01:01	Consensus (comb.lib./simm/nn)	MFFADDDSFYKYFAS	0.61	0.61
HLA-DRB3*01:01	Consensus (comb.lib./simm/nn)	FFADDDSFYKYFASQ	0.66	0.66
HLA-DRB5*01:01	Consensus (comb.lib./simm/nn)	FLLLLIQSKNKLEA	0.77	0.77
HLA-DRB1*03:01	Consensus (comb.lib./simm/nn)	NKVPIVTDGRVKLNK	0.78	0.78
HLA-DRB5*01:01	Consensus (comb.lib./simm/nn)	LLLLLIQSKNKLEAV	0.90	0.90
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	FNKVPIVTDGRVKLN	0.92	0.92
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	IVTDGRVKLNKGYLE	0.92	0.92
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	KVPIVTDGRVKLNKG	0.92	0.92
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	LFNKVPIVTDGRVKL	0.92	0.92
HLA-DRB1*03:01	Consensus (simm/nn/sturniolo)	PIVTDGRVKLNKGYLE	0.92	0.92

Table 3.13: Table of T-cell epitope prediction (MHC-II Binding Predictions) results of MPXV L1R monkeypox sequence.

5. IFNepitope Predictions

a) MPXV A33R

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

Table 3.14: Table of IFNepitope prediction results of MPXV A33R monkeypox sequence.

b) MPXV H3L

Epitope Name	Sequence	Method	Result	Score
Epitope1_H3L_	<u>LIVILFIMFMLIFNV</u>	SVM based	Positive	0.21168838
Epitope6_H3L_	<u>NDNVIEDITFLRPVL</u>	SVM based	Positive	0.59020904
Epitope9_H3L_	<u>LSAYIIRVTTALNIV</u>	SVM based	Positive	0.17927901
Epitope10_H3L_	<u>DNVIEDITFLRPVLK</u>	SVM based	Positive	0.63518805

Table 3.15: Table of IFNepitope prediction results of MPXV H3L monkeypox sequence.

c) MPXV M1R

Epitope Name	Sequence	Method	Result	Score
Epitope3_M1R_	<u>NFYIRQNHGCNITVK</u>	SVM based	Positive	0.19571364
Epitope4_M1R_	<u>AVVDNKLKIQNVIID</u>	SVM based	Positive	0.34328303
Epitope5_M1R_	LAALFMYAKRMLFT	SVM based	Positive	0.28389359
Epitope6_M1R_	VVDNKLKIQNVIIDE	SVM based	Positive	0.39634313
Epitope8_M1R_	GNFYIRQNHGCNITV	SVM based	Positive	0.43386317
Epitope9_M1R_	ILAALFMYAKRMLF	SVM based	Positive	0.054070519
Epitope10_M1R_	<u>AALFMYAKRMLFTS</u>	SVM based	Positive	0.61842338

Table 3.16: Table of IFNepitope prediction results of MPXV M1R monkeypox sequence.

d) MPXV L1R

Epitope Name	Sequence	Method	Result	Score
Epitope1_L1R_	MFFADDDSF F KYFAS	SVM based	Positive	0.036560014
Epitope3_L1R_	FLLLLLIQSKNKLEA	SVM based	Positive	0.18321976

Table 3.17: Table of IFNepitope prediction results of MPXV L1R monkeypox sequence.

6. Epitopes with Overlapping Residues

a) MPVX A33R

B-Cell Epitope	MCH-I Epitope	MCH-II Epitope	IFN Gamma Positive Score
FLEKTSFYNCN DSITKEKIK	R F EKTSFY	YNCYNYDDTFFDDDD	0.57336052
KVNNNNYNNYNNYN CYNNYNCY NYDDTFF	KV N NNNNY	NNYN C YNYDDTFFDD	0.36477612

Table 3.15: Table of epitopes with overlapping residues after IFNepitope prediction for MPXV A33R.

b) MPVX H3L

B-Cell Epitope	MCH-I Epitope	MCH-II Epitope	IFN Gamma Positive Score
PPSE T FPNVHEHIND QKFDDVKDNEVMQEK DVVIVNDDPDHY	E TFPNVHEHI	LIVILFIMFMLIFNV	0.21168838
ALWDSKFF T ELENKN	SLSAYIIRV	LSAYIIRV T TALNI	0.17927901
I TGNKVKTELVIDKDH	ITFLRPVLK	DNV I EDITFLRPVLK	0.63518805

Table 3.16: Table of epitopes with overlapping residues after IFNepitope prediction for MPXV H3L.

c) MPVX M1R

B-Cell Epitope	MCH-I Epitope	MCH-II Epitope	IFN Gamma Positive Score
KATTQI APROVAGT	APRQVAGT GV	IILAALFMYY A KRML	0.83197596
AALNIQTSVNTVVVRDF ENYVKQTCN	QTSVNTVVR	Q FYMIVIGVILAAL	0.69101888

Table 3.17: Table of epitopes with overlapping residues after IFNepitope prediction for MPXV M1R.

d) MPVX L1R

B-Cell Epitope	MCH-I Epitope	MCH-II Epitope	IFN Gamma Positive Score
KLEAVGHCHYESLS EEYRQLTK FTD SQDFKKLFNKVPIVTD	EEYRQLTKF	YLL T MFFADDDSF EK	0.18321976

Table 3.18: Table of epitopes with overlapping residues after IFNepitope prediction for MPXV L1R.

7. Docking with PatchDock

Ligand	Receptor	Solution Number	Global Energy	Attractive VdW	Repulsive VdW	ACE	HB
MPXV A33R	TLR4	1	-8.24	-12.52	12.78	3.94	-1.86
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.