

**Exploring dengue genome to construct a multi-epitope based subunit vaccine  
by utilizing immunoinformatics approach to battle against dengue infection**

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**Supplementary table 1:** Predicted CTL epitopes for structural and non-structural proteins of dengue virus

<b>S. No.</b>	<b>Protein</b>	<b>Sequence</b>	<b>Score</b>
1.	<b>prM</b>	TMMAAILAY	1.9915
2.		NSTSTWVTY	1.9773
3.		ELCEDTITY	1.1954
4.		MSSEGAWKH	0.9068
5.		TTEAELTGY	3.1769
6.		VVQPENLEY	2.1081
7.		QMSSGNLLF	1.3564
8.		QMENKAWLV	1.3366
9.		STSLSVTLV	1.2983
10.		VLVGIVTLY	1.0105
11.		GTIVIRVQY	0.9172
12.		KLQLKGMSY	0.8061
13.	<b>NS-1</b>	STESHNQTF	2.0681
14.		NVHTWTEQY	1.5861
15.		FTTNIWLKL	0.941
16.		ITDNVHTWT	0.929
17.		WNSLEVEDY	0.7769
18.	<b>NS-2A</b>	MTDDIGMGV	2.2165
19.		LTDALALGM	1.8278
20.		KTDWIPLAL	1.5206
21.		QVDNFSLGV	1.2211
22.		NMEKYQLAV	0.8604
23.		KMVRNMEKY	0.7628
24.	<b>NS-2B</b>	ITAAAWYLLW	0.786
25.	<b>NS-3</b>	KVDAIDGEY	2.7669
26.		YSQIGAGVY	2.6923
27.		KAELEDGAY	1.5754
28.		FTDPASIAA	1.4073
29.		RVAAEGINY	1.2975
30.		YSDPLALKE	1.2756
31.		LSPVRVPNY	1.1299
32.		VTDFKGKTV	0.9561
33.		GVVTRSGAY	0.9323
34.		RTNDWDFVV	0.782
35.		<b>NS-4A</b>	ITASILLWY
36.	TAEAGGRAY		1.3092
37.	<b>NS-4B</b>	VIDLDPIPY	1.7757
38.		LTAALFLLV	1.6802
39.		MANIFRGSY	1.4976
40.		YLAGAGLLF	1.1565
41.		ALFLLVAHY	0.7708

42.		TTLTAALFL	0.7589
43.	<b>NS-5</b>	YTDYMPSMK	2.2662
44.		ETACLGKSY	1.6863
45.		LINRFTMRY	1.6043
46.		RSLIGNEEY	1.5943
47.		FTDENKWKS	1.5825
48.		KTWAYHGSY	1.5116
49.		MTDTTPFGQ	1.2392
50.		YDQMWSLMY	1.1344
51.		KMEALQRKY	1.1153
52.		ASSMVNGVF	1.113
53.		MTTEDMLTV	1.1008
54.		LTSRATWAK	0.9451
55.		MSTYGWNLV	0.9043
56.		QEHETSWHY	0.8155
57.		FLEFEALGF	0.8038
58.		AEAIFKLTY	0.8019
59.		GSAKLRWFV	0.7776
60.		TTEDMLTVW	0.7598

**Supplementary table 2:** Predicted HTL epitopes for structural and non-structural proteins of dengue virus

<b>S.No.</b>	<b>Protein</b>	<b>Start and end position</b>	<b>Epitope</b>
1.	Protein C	39-59	QGRGPLKLYMALVAFLRFLTI
2.		69-85	WGTIKKSKAINVLRGFR
3.	prM	31-46	VNMCTLMAMDLGELCE
4.		85-100	EHRRQKRSVALVPHVG
5.		129-148	RHPGFTMMAAILAYTIGTTH
6.	Envelope	284-298	KCRLRMDKLQLKGMS
7.		406-422	MARGAKRMAILGDTAWDF
8.		439-465	VFGAIYGAAFSGVSWTMKILIGVIITW
9.	NS-1	28-53	WTEQYKFQPESPSKLASAIQKAHEEG
10.	NS-2A	51-66	RDLGRVMVMVGATMTD
11.		72-86	VTYLALLAAFKVRPT
12.		138-156	RNMEKYQLAVTIMAILCVP
13.	NS-2B	1-20	SWPLNEAIMAVGMVSILASS
14.		26-43	IPMTGPLVAGGPLTVCYV
15.	NS-3	2-16	GVLWDVPSPPPMGKA
16.		182-198	IFRKRRLTIMDLHPGAG
17.		261-279	CHATFTMRLLSVVRVFNYN
18.		437-453	GEERVILAGPMPVTHSS
19.	NS-4A	13-30	LPTFMTQKARDALDNLAV
20.		78-93	IGKMTLGMCCIITASI
21.		95-116	LWYAQIQPHWIAASIILEFFLI
22.	NS-4B	81-98	GWPLSKMDIGVPLLAIGC
23.		112-139	FLLVAHYAIIGPALQAKASREAQKRAAA
24.	NS-5	398-417	EFTRKVRNSNAALGAIIFTDEN
25.		609-626	LNTFTNMEAQLIRQMEGE

**Supplementary table 3:** Predicted B-cell epitopes for structural and non-structural proteins of dengue virus

S.No.	Protein	Position	Sequence	Score	
1.	<b>Protein C</b>	58	TIPPTAGILKRWGTIKKSKA	0.998	
2.		10	NTPFNMLKRERNRVSTVQQL	0.984	
3.	<b>prM</b>	59	NEPEDIDCWCNSTSTWVTYG	0.998	
4.		102	GLETRTETWMSSEGAWKHVQ	0.87	
5.		4	TTRNGEPHMIVSRQEKGKSL	0.836	
6.	<b>Envelope</b>	382	VEPGQLKLNWFKKGSSIGQM	1	
7.		217	PLPWLPGADTQGSNWIQKET	0.994	
8.		64	KLTNTTTESRCPTQGEPSLN	0.992	
9.		353	TVNPIVTEKDSPVNIEAEP	0.987	
10.		317	HGTIVIRVQYEGDGSPCKIP	0.978	
11.		152	GNDTGKHGKEIKITPQSST	0.976	
12.		96	MVDRGWGNGCGLFGKGGIVT	0.914	
13.		119	FRCKKNMEGKVVQPENLEYT	0.886	
14.		175	LTGYGTVTMECSPRTGLDFN	0.869	
15.		43	FELIKTEAKQPATLRKYCIE	0.849	
16.		241	KNPHAKKQDVVVLGSQEGAM	0.813	
17.		22	DIVLEHGSCVTTMAKNKPTL	0.803	
18.		<b>NS-1</b>	105	RPQPTTELKYSWKTWGKAKML	1
19.			293	NRGPLRRTTASGKLITEWC	0.992
20.			325	GEDGCWYGMEIRPLKEKEEN	0.992
21.	135		IDGPETAECPTNRAWNSLE	0.988	
22.	243		IPKNLAGPVSQHNYRPGYHT	0.976	
23.	22		TDNVHTWTEQYKFQPESPSK	0.877	
24.	84		VKLTIMTGDIKGIMQAGKRS	0.851	
25.	<b>NS-2B</b>		79	SEDGSMSIKNEEEEQTLTIL	1
26.		23	KNDIPMTGPLVAGGPLTVCY	0.947	
27.	<b>NS-3</b>	569	NNQILEENVEVEIWTKEGER	1	
28.		129	DFSPGTSGSPIIDKKGKVVG	0.999	
29.		312	IFMTATPPGSRDPFPQSNAP	0.998	
30.		102	PGKNPRAVQTKPGLFKTNAG	0.992	
31.		78	SYGGGWKLEGEWKEGEEVQV	0.987	
32.		5	WDVPSPPPMGKAELEDGAYR	0.978	
33.		334	DEEREIPERSWNSGHEWVTD	0.965	
34.		167	QTEKSIEDNPEIEDDIFRKR	0.928	
35.		387	RKTFDSEYAKTRTNDWDFVV	0.923	
36.		456	QRRGRIGRNPNKNENDQYIYM	0.89	
37.		496	DNINTPEGIIPSMFEPEREK	0.859	
38.		527	GEARTTFVDLMRRGDLPVWL	0.855	

39.		435	TDGEERVILAGPMPVTHSSA	0.826
40.	<b>NS-4B</b>	197	ATGPISTLWEGNPGRFWNTT	0.995
41.		151	TVIDLDPIPYDPKFEKQLGQ	0.846
42.	<b>NS-5</b>	101	KGLTKGGPGHEEPIPMSTYG	1
43.		878	EYTDYMPSMKRFRREEEEAG	0.998
44.		524	KKEGGAMYADDTAGWDTRIT	0.997
45.		575	NKVVRVQRPTPRGTVMDIIS	0.997
46.		819	QENPW MEDKTPVESWEEIPY	0.997
47.		144	LCDIGESSPNPTVEAGRTRLR	0.993
48.		380	WLWKELGKKKTPRMCTREEF	0.974
49.		351	QQRVFKEKVDTRTQEPKEGT	0.964
50.		329	TKPWDVVPMTQAMTDTP	0.96
51.		682	NDTGKIRKDIQQWEP SRGWN	0.958
52.		165	LNLVENWLNNTQFCIKVLN	0.953
53.		20	LGKSEFQIYKKSIGQEVDR	0.943
54.		304	AYHGSYETKQTGSASSMVNG	0.937
55.		457	KREKKLGEFGKAKGSRAIY	0.936
56.		283	KIKQEHETSWHYDQDHPYKT	0.926
57.		781	SAVPSHWVPTSRTTWSIHAK	0.921
58.		243	FTMRYKKATYEPDVLGSGT	0.891
59.	215	THEMYWVSNASGNIVSSVNM	0.807	

**Supplementary table 4:** Interferon  $\gamma$  inducing epitopes for final vaccine construct predicted using IFNepitope server

S.No.	Start-End	Sequence	Score
1.	7—22	QYAAWNSLEVEDYA	2
2.	8—23	YAAWNSLEVEDYAA	2
3.	9—24	AAWNSLEVEDYAA	2
4.	10—25	AWNSLEVEDYAA	2
5.	11—26	WNSLEVEDYAA	2
6.	12—27	NSLEVEDYAA	2
7.	13-28	NSLEVEDYAA	2
8.	14-29	SLEVEDYAA	2
9.	15-30	LEVEDYAA	2
10.	16-31	EVEDYAA	2
11.	17-32	VEDYAA	2
12.	18-33	EDYAA	2
13.	48-63	KVDAIDGEYAA	1
14.	49-64	VDAIDGEYAA	1
15.	50-65	DAIDGEYAA	1
16.	85-100	IDLPIPYAA	1
17.	86-101	DLPIPYAA	1
18.	87-102	LDPIPYAA	1
19.	88-103	DPIPYAA	1
20.	89-104	PIPYAA	1
21.	90-105	IPYAA	1
22.	91-106	PYAA	1
23.	92-107	YAA	1
24.	133-148	STYGWNLVAA	1
25.	134-149	TYGWNLVAA	1
26.	135-150	YGWNLVAA	1
27.	136-151	GNLVAA	1
28.	137-152	WNLVAA	1
29.	138-153	NLVAA	1
30.	139-154	LVA	1
31.	140-155	VAA	1
32.	141-156	AA	1
33.	157-172	SSEGAWKHA	1
34.	158-173	SEGAWKHA	1
35.	159-174	EGAWKHA	1
36.	160-175	GAWKHA	3
37.	161-176	AWKHA	5
38.	162-177	WKHA	5

39.	163-178	KHAAYTTEAELTGYA	4
40.	164-179	HAAYTTEAELTGYAA	4
41.	165-180	AAYTTEAELTGYAAY	4
42.	166-181	AYTTEAELTGYAAYV	4
43.	167-182	YTTEAELTGYAAYVV	4
44.	236-251	GVTYLALLAAFKVRP	1.00042
45.	289-304	MDLHPGAGGPGPGGV	1.187181
46.	290-305	DLHPGAGGPGPGGVL	1.200201
47.	291-306	LHPGAGGPGPGGVLW	1.15008
48.	292-307	HPGAGGPGPGGVLWD	1.119006
49.	293-308	PGAGGPGPGGVLWDV	1.038983
50.	336-351	QAKASREAQKRAAAG	1
51.	337-352	AKASREAQKRAAAGP	1
52.	338-353	KASREAQKRAAAGPG	1
53.	352-367	GPGWTEQYKFQPESP	1
54.	353-368	PGWTEQYKFQPESPS	1
55.	355-370	WTEQYKFQPESPSKL	1
56.	356-371	TEQYKFQPESPSKLA	1
57.	357-372	EQYKFQPESPSKLAS	1
58.	358-373	QYKFQPESPSKLASA	1

**Supplementary table 5:** GalaxyRefine score of all predicted refined models

<b>Model</b>	<b>GDT-HA</b>	<b>RMSD</b>	<b>MolProbity</b>	<b>Clash score</b>	<b>Poor Rotamer</b>
<b>Initial</b>	<b>1.0000</b>	<b>0.000</b>	<b>3.646</b>	<b>128.7</b>	<b>4.1</b>
MODEL 1	0.9261	0.478	2.396	28.3	0.6
MODEL 2	0.9240	0.480	2.619	29.5	1.8
MODEL 3	0.9207	0.483	2.588	29.9	1.5
MODEL 4	0.9163	0.496	2.447	26.9	1.2
MODEL 5	0.9158	0.501	2.471	30.8	0.6