ACCSCIENCE PUBLISHING

Microbes & Immunity

ORIGINAL RESEARCH ARTICLE

An *in silico* approach to design a multi-epitope vaccine against small ruminant lentiviruses causing Maedi-Visna and caprine arthritis encephalitis in sheep and goats

Supplementary File

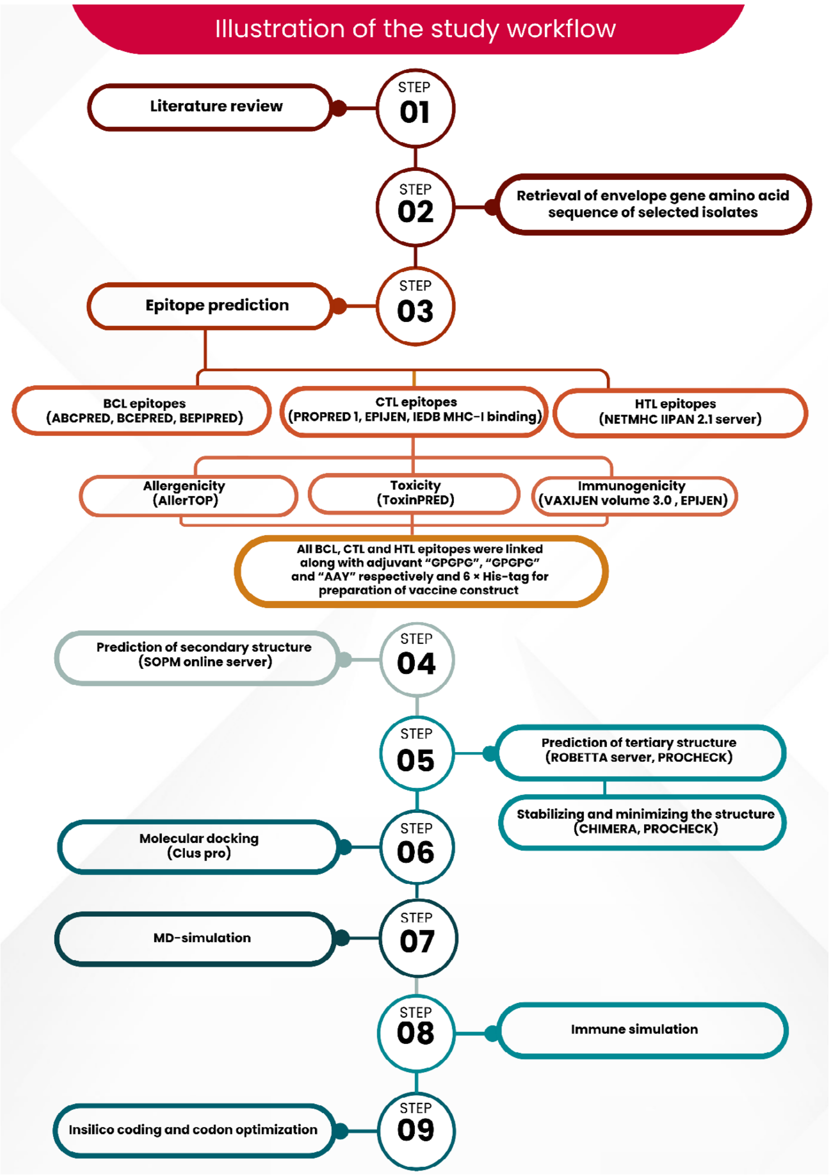

Figure S1. Study design for the small ruminant lentivirus-based vaccine candidate against Maedi-Visna virus and caprine arthritis encephalitis virus in sheep and goats

Abbreviations: BCL: B cell lymphocyte; CTL: Cytotoxic T lymphocyte; HTL: Helper T lymphocyte.

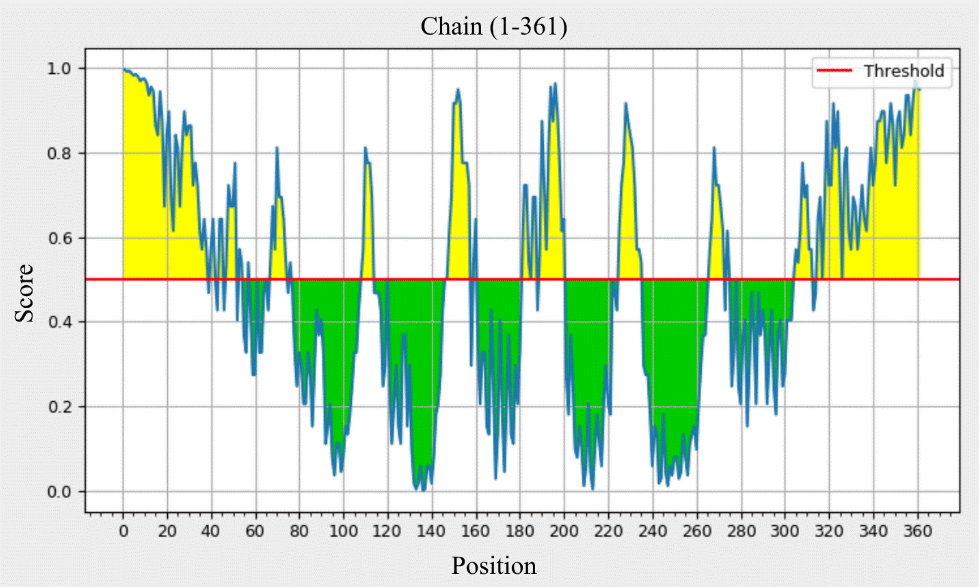

Figure S2. Prediction of the discontinuous T-cell epitopes for the small ruminant lentivirus vaccine construct. The scores for the discontinuous B-cell epitopes were calculated using the ElliPro web server. The X-axis shows the positions of the residues, whereas the scores for each residue are depicted on the Y-axis.

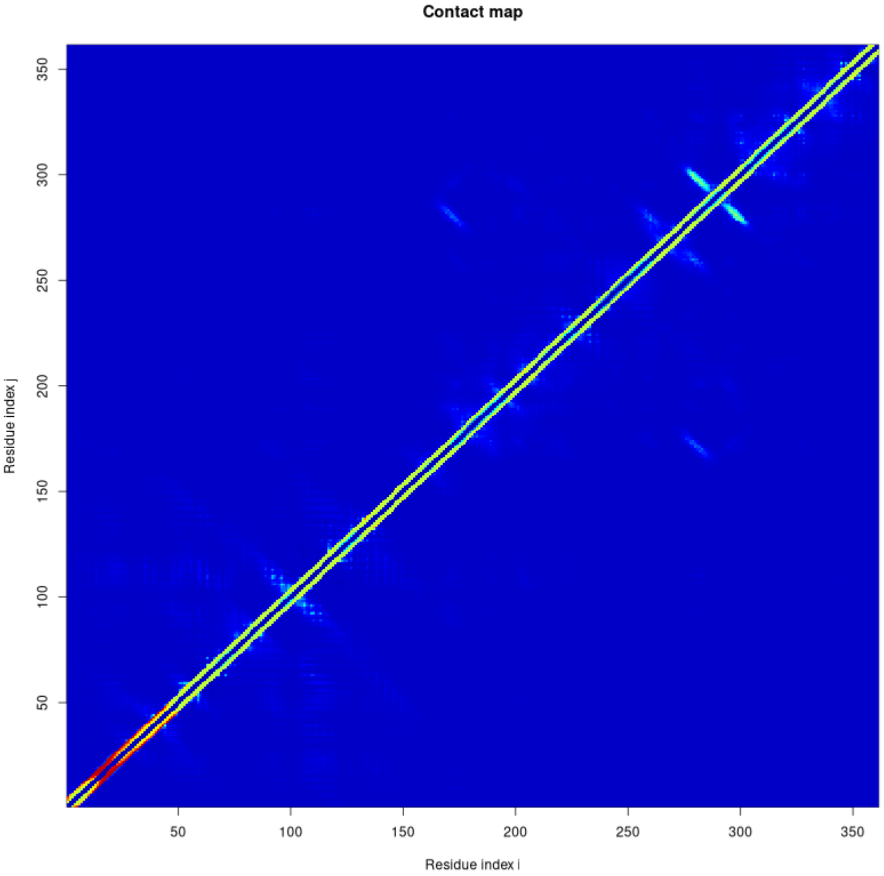

Figure S3. Contact map analysis for the small ruminant lentivirus-based vaccine construct. The different contact points present in the generated vaccine construct were obtained using the PSIPRED tool.

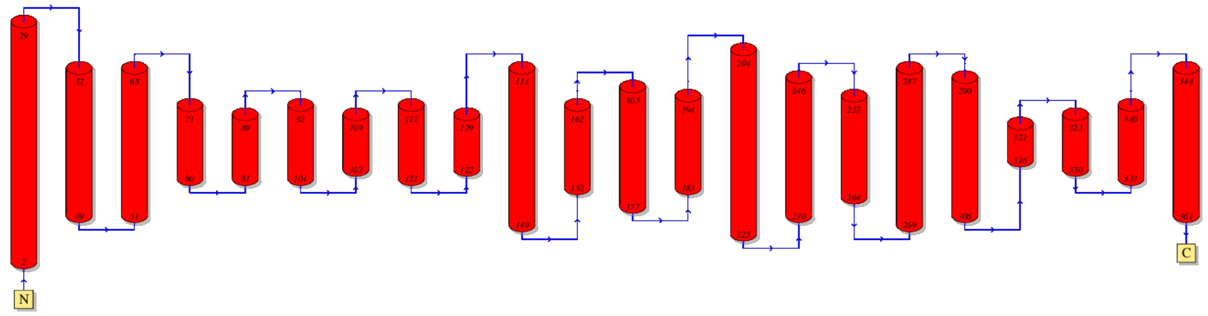

Figure S4. Analysis for the tertiary structure of the small ruminant lentivirus-based vaccine candidate. The refined three-dimensional structure of the vaccine construct model was analyzed using the PROCHECK web server.

Table S1. Prediction of discontinuous B-cell epitopes

No.	Residues	Number of residues	Score
1	A:M1, A:G2, A:K3, A:K4, A:K5, A:C6, A:S7, A:K8, A:S9, A:A10, A:E11, A:A12, A:A13, A:A14, A:K15, A:S16, A:M17, A:M18, A:H19, A:Q20, A:Q21, A:M22, A:L23, A:L24, A:A25, A:A26, A:R28, A:Q29, A:Q30, A:E31, A:Q32, A:E33, A:K34, A:L35, A:L36, A:A37, A:A38, A:R40, A:Q41, A:Q42, A:Q44, A:E45, A:I53, A:A54, A:K57, A:E61, A:K65, A:K69, A:S70, A:M71, A:E72, A:P73, A:P74, A:R76	54	0.768
2	A:G304, A:K305, A:K306, A:G307, A:K308, A:G309, A:P310, A:G311, A:P312, A:G313, A:N314, A:C315, A:S316, A:L317, A:P318, A:H319, A:I320, A:N321, A:E322, A:S323, A:S324, A:K325, A:W326, A:T327, A:C328, A:A329, A:G330, A:P331, A:G332, A:P333, A:G334, A:D335, A:R336, A:T337, A:G338, A:N339, A:G340, A:A341, A:L342, A:G343, A:N344, A:V345, A:K346, A:N347, A:K348, A:N349, A:C350, A:E351, A:A352, A:A353, A:A354, A:K355, A:H356, A:H357, A:H358, A:H360, A:H361	57	0.739
3	A:V109, A:I110, A:Q111, A:M112, A:V113, A:Y146, A:M147, A:E148, A:A149, A:Q150, A:G151, A:E152, A:N153, A:R154, A:R155, A:S156, A:R157, A:N159, A:L160	19	0.73
4	A:G179, A:G180, A:L181, A:D182, A:G183, A:P184, A:G185, A:P186, A:G187, A:L189, A:L190, A:G191, A:T192, A:E193, A:R194, A:G195, A:E196, A:E197, A:K198, A:Q199, A:K200	21	0.677
5	A:L47, A:L48, A:A49, A:A50, A:Y51	5	0.677
6	A:G222, A:G225, A:P226, A:G227, A:P228, A:G229, A:Q230, A:Q231, A:E232, A:Q233, A:E234, A:K235, A:P266, A:G267, A:P268, A:G269, A:P270, A:G271, A:E272, A:K274, A:Q275, A:W278	22	0.675
7	A:Y27, A:T67, A:W68, A:W108	4	0.632

Table S2. Self-optimized prediction method (SOPMA)

Structure	No of residues	Percentage	Impact on structure
Alpha helix	94	26.04%	Provides functional adaptability at various structural configurations, flexibility, stability, and rigidity to the structure
3_{10} helix	0	0.00%	Appears as an intermediate structure before a stable loop formation, often found involved in amino acid binding pocket regions
Pi helix	0	0.00%	As a rare and functional protein, it plays a major role by creating structural distortions, enabling specialized functions within the protein and facilitating active-site geometry.
Beta bridge	0	0.00%	Contributes to the overall orientation of protein by connecting β-strands into sheets and exposing residues that play a role in binding and recognition due to tight and stable turns
Extended strands	66	18.28%	Plays a vital role in protein interactions

(Cont'd...)

Table S2. (*Continued*)

Structure	No of residues	Percentage	Impact on structure
Beta turn	0	0.00%	Facilitates the polypeptide chain to fold back on itself, which ultimately increases flexibility, reduces the overall length or size, forming a compact structure
Bend region	0	0.00%	Promotes the formation of the proper three-dimensional structure of the protein by redirecting the backbone, along with enhancing the structure's flexibility
Random coil	201	55.68%	Allows evolutionary changes in protein structure without damaging it by providing movement, stability, and adaptability, serving as a functional binding site.
Ambiguous states	0	0.00%	Plays dynamic roles in protein regulation and signaling, along with conformational changes due to protein folding, which provide structural flexibility
Other states	0	0.00%	Improves the overall broad range of protein functions

Note: This table indicates the structural components, their abundance, and their impact on the secondary structure.

Table S3. Galaxy Refine scores for I-TASSER models

Model	GDT-HA	RMSD	MolProbity	Clash score	Poor rotamers	Ramachandran favored residues (%)
Initial	1.0000	0.000	4.826	325.8	52.0	89.7
Model 1	0.9515	0.393	2.113	21.4	0.4	95.8
Model 2	0.9626	0.378	2.483	23.9	2.5	95.5
Model 3	0.9557	0.402	2.339	20.1	1.8	95.0
Model 4	0.9578	0.383	2.347	20.3	2.5	96.4
Model 5	0.9536	0.401	2.137	21.4	1.1	95.8

Note: This table lists the five models and their Galaxy Refine scores, obtained after uploading the best I-TASSER model.
Abbreviations: GDT-HA: Global distance test–high accuracy; RMSD: Root mean square deviation.

Table S4. Cluster scores by ClusPro for the TLR-4 (4G8A) and vaccine construct docked model

Cluster	Members	Representative	Weighted score
0	95	Center	−925.0
		Lowest energy	−1,221.7
1	58	Center	−913.0
		Lowest energy	−1,090.8
2	46	Center	−1,031.8
		Lowest energy	−1,113.0
3	42	Center	−1,003.2
		Lowest energy	−1,089.2
4	39	Center	−998.3
		Lowest energy	−1,234.9
5	37	Center	−902.4
		Lowest energy	−1,080.9
6	37	Center	−984.1
		Lowest energy	−1,081.9

(*Cont'd...*)

Table S4. (*Continued*)

Cluster	Members	Representative	Weighted score
7	35	Center	−1,063.1
		Lowest energy	−1,089.3
8	35	Center	−948.0
		Lowest energy	−1,070.8
9	32	Center	−1,004.8
		Lowest energy	−1,112.8
10	30	Center	−1,003.7
		Lowest energy	−1,017.5
11	27	Center	−991.7
		Lowest energy	−1,111.4
12	26	Center	−937.9
		Lowest energy	−1,031.0
13	26	Center	−954.6
		Lowest energy	−1,044.0
14	25	Center	−915.0
		Lowest energy	−1,080.5
15	25	Center	−1,078.8
		Lowest energy	−1,126.3
16	19	Center	−958.9
		Lowest energy	−1,041.2
17	18	Center	−936.9
		Lowest energy	−970.4
18	16	Center	−902.0
		Lowest energy	−1,201.9
19	15	Center	−897.1
		Lowest energy	−1,062.8
20	13	Center	−1,111.4
		Lowest energy	−1,111.4
21	13	Center	−954.4
		Lowest energy	−1,081.4
22	12	Center	−947.1
		Lowest energy	−963.6
23	12	Center	−1,070.3
		Lowest energy	−1,070.3
24	11	Center	−938.6
		Lowest energy	−983.7
25	11	Center	−954.6
		Lowest energy	−954.6

(*Cont'd...*)

Table S4. (*Continued*)

Cluster	Members	Representative	Weighted score
26	10	Center	−1,018.8
		Lowest energy	−1,035.3
27	9	Center	−953.3
		Lowest energy	−1,050.3
28	9	Center	−943.8
		Lowest energy	−1,043.7
29	9	Center	−907.2
		Lowest energy	−1,116.2

Notes: This table provides information on the number of clusters generated by ClusPro and the number of members in each. The cluster center value and the lowest-energy value for each cluster are given in their respective rows.

Table S5. Cluster scores by ClusPro for the TLR-2 (6NIG) and vaccine construct docked model

Cluster	Members	Representative	Weighted score
0	62	Center	−1,030.9
		Lowest energy	−1,170.6
1	56	Center	−1,151.4
		Lowest energy	−1,151.4
2	48	Center	−894.0
		Lowest energy	−1,035.7
3	41	Center	−1,123.7
		Lowest energy	−1,158.1
4	35	Center	−958.2
		Lowest energy	−1,021.3
5	33	Center	−930.9
		Lowest energy	−939.2
6	26	Center	−950.6
		Lowest energy	−950.6
7	22	Center	−996.0
		Lowest energy	−1,071.2
8	19	Center	−980.3
		Lowest energy	−980.3
9	18	Center	−972.0
		Lowest energy	−972.0
10	17	Center	−1,086.8
		Lowest energy	−1,086.8
11	17	Center	−1,011.9
		Lowest energy	−1,011.9
12	16	Center	−1,042.8
		Lowest energy	−1,042.8

(*Cont'd...*)

Cluster	Members	Representative	Weighted score
13	16	Center	−993.5
		Lowest energy	−993.5
14	16	Center	−950.6
		Lowest energy	−950.6
15	15	Center	−1,164.1
		Lowest energy	−1,164.1
16	15	Center	−1,007.0
		Lowest energy	−1,007.0
17	13	Center	−969.8
		Lowest energy	−969.8
18	12	Center	−892.0
		Lowest energy	−911.0
19	12	Center	−913.5
		Lowest energy	−913.5
20	12	Center	−903.3
		Lowest energy	−908.9
21	12	Center	−857.1
		Lowest energy	−919.6
22	11	Center	−1,115.8
		Lowest energy	−1,115.8
23	11	Center	−936.7
		Lowest energy	−936.7
24	10	Center	−1,013.3
		Lowest energy	−1,013.3
25	10	Center	−871.6
		Lowest energy	−939.6
26	9	Center	−859.6
		Lowest energy	−950.3

Notes: This table provides information on the number of clusters generated during protein-protein docking for the SRLV vaccine construct and the 6NIG protein-ligand complex using ClusPro, along with the number of members in each cluster. The cluster center value and the lowest-energy value for each cluster are given in the rows corresponding to each cluster.