

Supplementary file 1

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In silico prediction of vaccine and diagnostic epitopes in *Bartonella henselae* MopA, VceA, and LemA proteins

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Table S1: Properties of selected B-cell, MHC-I and MHC-II epitopes.

B-cell Epitopes							
Protein	Epitope			Antigenicity value		Solubility	Allergenicity
				VaxiJen	VaxiGen		
MopA	KEVKFGREARERLLRG			0.4346	Immunogen (100%)	Good water solubility	Non-Allergen
VceA	APQSDVDDAKSAYE			0.8763	Immunogen (100%)	Good water solubility	Non-Allergen
MHC-I Epitopes							
Protein	Allele	Peptide	EL percentile	Antigenicity value		Solubility	Allergenicity
				VaxiJen	VaxiGen		

MopA	HLA-B*08:01 HLA-A*26:01	EINARVNQI	0.2 0.49	1.6135	Immunogen (66%)	Good water solubility	Non-allergen
	HLA-A*03:01	RAANALTVK	0.23	1.5129	Immunogen (66%)	Good water solubility	Non-allergen
	HLA-A*26:01	ENNADTFGY	0.43	0.775	Immunogen (100%)	Good water solubility	Non-allergen
	HLA-B*08:01	ELEDKFENM	0.5	0.5673	Immunogen (100%)	Good water solubility	Non-allergen
VceA	HLA-B*27:05	KRIRAGMSV	0.12	0.9774	Immunogen (66%)	Good water solubility	Non-allergen
	HLA-A*03:01	SVQIDTRTK	0.32	1.6781	Immunogen (100%)	Good water solubility	Non-allergen
	HLA-B*39:01	TRDKAKRDL	0.32	1.0156	Immunogen (66%)	Good water solubility	Non-allergen
	HLA-A*03:01	KSLELTRDK	0.47	0.4247	Immunogen (100%)	Good water solubility	Non-allergen
MHC-II Epitopes							

Protein	Allele	Peptide	EL percentile	Antigenicity value		Solubility	Allergenicity
				VaxiJen	VaxiGen		
MopA	HLA-DRB1*03:01	APRITKDGVSVAKEI	0,66	0.6119	Immunogen (100%)	Good water solubility	Non-allergen
	HLA-DRB3*02:02	RQIATNAGEEAAIIV	0,9	0.4801	Immunogen (100%)	Good water solubility	Non-allergen
	HLA-DRB3*01:01	TSGQVISEDVGIKLE	1,2	1.4163	Immunogen (100%)	Good water solubility	Non-allergen
VceA	HLA-DRB5*01:01	AGQTAYITFDAFKKE	0.13	0.4227	Immunogen (66%)	Good water solubility	Non-allergen
	HLA-DRB1*15:01 HLA-DRB3*02:02 HLA-DRB5*01:01	KKIAIKANQVVKKDD	0.5 0.6 1.3	0.9072	Immunogen (66%)	Good water solubility	Non-allergen

Bold residues indicate non-linear B-cell epitopes predicted by ElliPro, whereas underlined residues also indicate non-linear B-cell epitopes predicted by BepiPred 3.0. Default threshold values were used during BCEPRED, ElliPro, and BepiPred analyses. The threshold value for VaxiJen was 0.4. The EL percentile value for MHC-I was < 0.5, while the EL percentile value for MHC-II was < 2. Twelve HLA class I super-type (A*01:01, A*02:01, A*03:01, A*24:02, A*26:01, B*07:02, B*08:01, B*27:05, B*39:01, B*40:01, B*58:01, and B*15:01) and seven HLA class II reference set (DRB1*03:01, DRB1*07:01, DRB1*15:01, DRB3*01:01, DRB3*02:02, DRB4*01:01, and DRB5*01:01) were used to predict MHC-I and MHC-II epitopes.

Table S2: Physico-chemical, antigenicity and transmembrane properties of the vaccine construct

Properties	Vaccine
Amino acids	271
Molecular weight (MW)	28287.30
Theoretical pI	9.33
Negatively charged residues (Asp+Glu)	30
Positively charged residues (Arg+Lys)	37
Estimated half-life (<i>E. coli</i>)	>10 hours
Instability index	16.57/Stable
Aliphatic index	67.20
GRAVY	-0.544
Antigenicity(Vaxijen/VaxiGen)	0.9283/Immunogen (100%)
*Solubility	0.678/Soluble
Number of predicted TMHs	None
Allergenicity	Non-Allergen

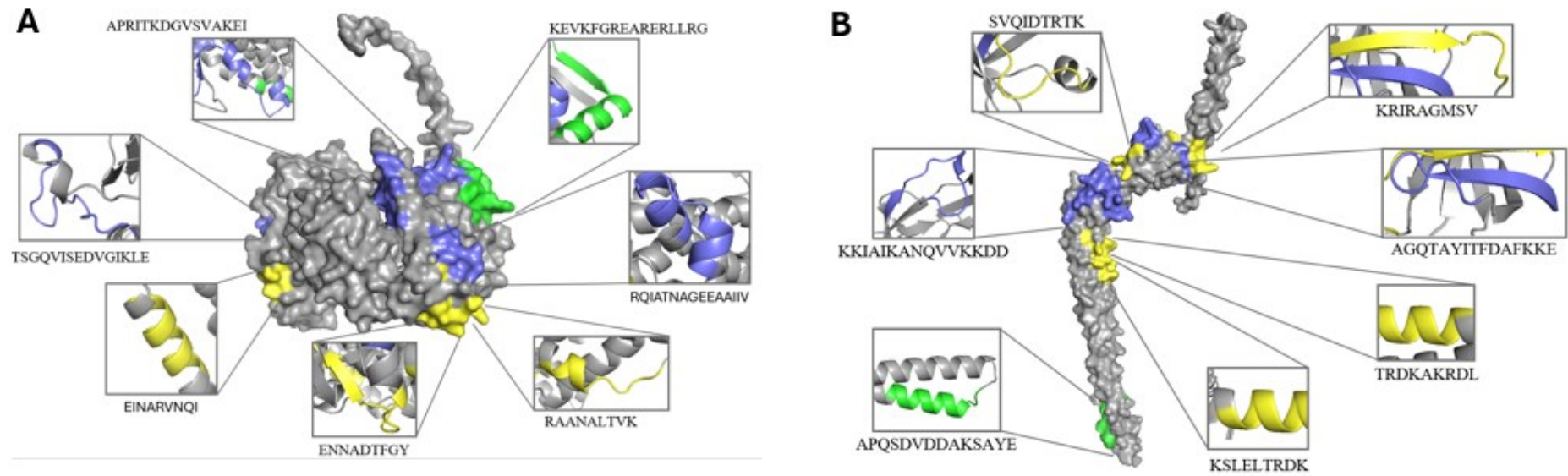


Figure S1: Structural mapping of selected epitopes on the 3D structures of the MopA and VceA proteins. A) Visualization of selected epitopes on the MopA protein. B) Visualization of selected epitopes on the VceA protein. B-cell epitopes are shown in green, MHC-I epitopes in yellow, and MHC-II epitopes in blue.