In silico analysis of a new *Brucella* vaccine candidate

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Abstract: Vaccination against *Brucella* spp. play an important role in brucellosis control and eradication program, worldwide [1]. Approved vaccines strains commonly used to animal protection against brucellosis infection, however, due to some disadvantages shown by these vaccines, effort has been undergone for the development of new vaccine with more efficacy and safety that could be used also in other animals and human [2]. In this study, we evaluated the immune responses -*in silico*- induced by a designed recombinant chimera protein as a novel *Brucella* vaccine candidate. Three antigens of *Brucella* have been structures *in silico*, as potential immunogenic antigens (trigger factor-TF, Omp31 and Bp26) and were fused together by EAAAK linkers to designe a chimera [3]. The sequences of components were aligned using multiple sequence alignment software (http://workbench.sdsc.edu/). Signal peptide location and transmembrane regions were determined using SignalP and TMAP servers, respectively. Antigenicity of protein were determined by Immune Epitope Database (IEDB) analysis resource (http://www.iedb.org). The physicochemical parameters were determined using ProtParam server (http://us.expasy.org/tools/protparam.html). Protein secondary and tertiary structures were predicted using GOR4 (https://npsa-prabi.ibcp.fr/cgi-bin/npsa) and I-TASSER (http://zhanglab.ccmb.med.umich.edu/I-TASSER) servers, respectively. Energy minimization for the three dimensional (3D) models was performed using Swiss-PDB Viewer 4.1 software. Analysis of the 3D model was made using protein structure analysis (ProSa) server (https://prosa.services.came.sbg.ac.at/prosa.php) and Ramachandran Plot Analysis resource (RAMPAGE). The Z-score (overall model quality) and energy plots were created by ProSa server. T-cell epitope prediction (IEDB T-cell epitope prediction tools were used for identification of MHC II epitopes). Prediction of antigenic B-cell epitopes (BCPred server was used for prediction of continuous B-cell epitopes). Prediction of discontinuous B-cell epitopes from 3D protein structure was performed using ElliPro antibody epitope prediction tool [4]. Finally, our results shown that this recombinant chimeric protein could be a potential antigen candidate for the development of a subunit vaccine against *Brucella* according to Bioinformatics results.

Keywords: *Brucella*, Vaccine, Immunity and Recombinant

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