Computational prediction of B-cell linear epitopes from Wb14: a *Wuchereria bancrofti* antigen used for the serodiagnosis of lymphatic filariasis

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Lymphatic filariasis is an endemic tropical and subtropical parasitosis which affects 50 million people worldwide and is caused by *Brugia malayi*, *B. timori*, and mainly by *Wuchereria bancrofti*. Some countries, including Brazil, are in the surveillance phase of the Global Program for the Elimination of Lymphatic Filariasis (GPELF), which aims to eliminate the disease. The main antibody-capture tests used for its diagnosis, Wb123 and Bm14, are imported and based on antigens from *W. bancrofti* and *B. malayi*, respectively. Previous studies investigated Wb14, an orthologue of Bm14, for its potential use in anti-*W. bancrofti* antibody detection tests. The present work aimed to predict the three-dimensional structure of the Wb14 antigen and computationally identify its B cell epitopes. The Wb14 coding sequence was retrieved from GenBank (accession number: AAC17637.1). The three-dimensional structure of the Wb14 antigen was computationally predicted using Alphafold2. The predicted structure was refined by restrained energy minimization with AMBER and validated by analyzing the phi and psi residue angles using PROCHECK. B cell epitopes were predicted from the structural model of the Wb14 protein using the Ellipro software. In addition, the antigenicity of the predicted epitopes was evaluated using the VaxiJen v2 software. The three-dimensional model of the Wb14 antigen presented a predicted template modeling (pTM) score of 0.74 and a mean confidence value (pLDDT) of 83.22. Furthermore, 132 residues (95.7 %) have phi and psi angles in the most favored regions, while six residues (4.3%) have angles in additionally allowed regions. A total of five epitopes were identified from the computationally predicted model. Three of those were predicted to be highly antigenic, with scores of 1.82, 2.35, and 1.00. Two others were predicted to have a mild antigenicity, with scores of 0.01 and 0.11. The computational analysis carried out here is an important first step towards the solving of the three-dimensional structure of the Wb14 protein. It also facilitates the elucidation of the molecular basis responsible for its antigenicity. This knowledge should also be useful for the optimization of serological methods applied to the diagnosis of lymphatic filariasis based on the Wb14 antigen, since the identified B cell epitopes can be included in a synthetic multiepitope chimeric antigen designed specifically with this aim.

Keywords: Immunoinformatics; ELISA; immunodiagnostic.