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Epitope prediction, modeling, and docking studies for H3L protein as an agent of smallpox

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Abstract

Despite the eradication of *Variola* and *Vaccinia viruses*, smallpox is still a potential threat to human societies. The H3L protein is conserved and immune-dominant among different strains of poxviruses. The aim of this study was to detect epitope regions in the H3L protein by bioinformatics tools and examine the accuracy of an experimentaly determined epitope, VP35#1, against HLA-A*0201 by molecular docking. H3L epitopes were predicted against major histocompatibility complex (MHC) II receptors by bioinformatics servers. Antigenic potency of these epitopes was investigated using Vaxijen 2.0 software. The digestibility of predicted epitopes was predicted using online servers. Epitopes that were missed in the partial crystallographic structure of H3L protein were modeled using Muster server. It has been determined that H3L protein, including 8 predicted epitopes for 6 MHC Class II receptors, is conserved among the agents of smallpox. The antigenicity of the epitopes has been confirmed through Vaxijen 2.0 software. The binding affinity for docking VP35#1 and the HLA-A*0201 receptor ($-\Delta G = -7.4$) showed stable and powerful interaction.

Key words: bioinformatics, receptor, MHC II, epitope, smallpox, H3L protein

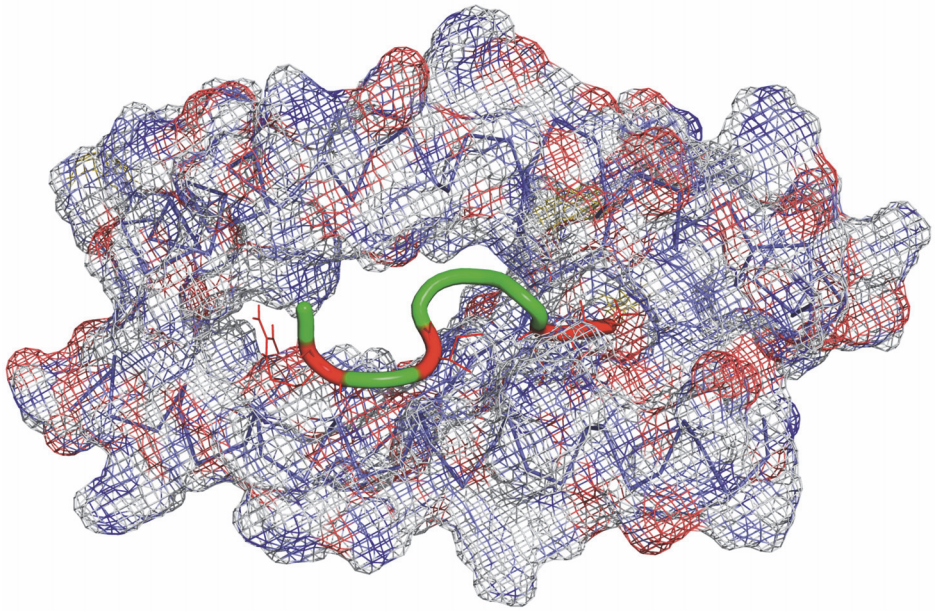

Fig. S1. Positioning the VP35#1 epitope (colored in red and green) in the binding groove of HLA A*0201 allele as an MHC I receptor. The residues of the epitope interacting with side chains of the receptor are colored in red. Only the binding groove of the receptor is shown

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