



Design and Molecular Docking Study of Recombinant Chimera Protein HBHA-Omp28 for Developing an Efficient Vaccine Against *Salmonella typhimurium*

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Abstract

BACKGROUND: Salmonellosis is a dangerous disease that can threaten the health of humans and animals. This disease can lead to economic losses annually; therefore, many studies have been conducted to prevent this disease.

OBJECTIVES: The current study aims to design a recombinant chimera protein HBHA-Omp28 as a vaccine against *Salmonella typhimurium*.

METHODS: The nucleotide and amino acid sequences of Omp28 and HBHA proteins were first extracted from the NCBI database. Then, the recombinant chimera of HBHA-Omp28 was bioinformatically assembled using a rigid linker. Epitope prediction of T and B cells, antigenicity, allergenicity, and physicochemical features assessments of HBHA-Omp28 were done using Immune Epitope Database (IEDB), ABCpred, VaxiJen, AllerTOP and ProtParam online servers, respectively. To assess the secondary and tertiary structures, the Self-Optimized Prediction Method with Alignment (SOPMA) and the Iterative Threading ASSEMBLY Refinement (I-TASSER) server were used, respectively. Molecular docking between recombinant chimera and TLR4/MD2 receptor was assessed by ClusPro server. Finally, after codon optimization of nucleotide sequence of recombinant chimera to express in *Escherichia Coli* k-12 strain, the cloning of recombinant chimera in pET21-a (+) vector was examined.

RESULTS: The designed recombinant chimera was classified as an antigenic and non-allergenic protein with molecular weight of 34.19 kDa. According to the results of molecular docking study, the HBHA-Omp28 protein was able to bind to TLR4/MD2 receptor using 9 hydrogen bonds. The results of cloning study demonstrated that HBHA-Omp28 successfully cloned into pET21-a (+).

CONCLUSIONS: The designed recombinant chimera can be an appropriate vaccine against salmonella bacteria.

Keywords: Bioinformatics, Salmonellosis, Recombinant protein, Infection, Vaccination

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Figure Legends and Table Captions

Table 1. List of predicted epitopes using IEDB and ABCpred servers and their antigenicity.

Table 2. List of effective amino acids involved in hydrogen bonds formation.

Figure 1. Final structure of HBHA-Omp28.

Figure 2. Secondary structure of HBHA-Omp28 obtained by the SOPMA.

Figure 3. Ramachandran plot of HBHA-Omp28 before refinement. In this model, 260 (82%) residues were located in the core area.

Figure 4. Ramachandran plot of HBHA-Omp28 after refinement. In this model, 288 (91%) residues were located in the core area.

Figure 5. The best refined model of HBHA-Omp28, visualized by PyMol software.

Figure 6. Interaction between HBHA-Omp28 protein and TLR4/MD2 receptor.

Figure 7. Number and length of hydrogen bonds between HBHA-Omp28 protein and TLR4/MD2 receptor visualized by LigPlot+ software.

Figure 8. Cloning the nucleotide sequence of HBHA-Omp28 (green color) into pET21-a (+) vector.