University of Tehran Press

Journal of Veterinary Research

Homepage: jvr.ut.ac.ir

Online ISSN: 2251-6190

Original Article

J Vet Res, Volume 78, Number 3, 2023, 223-233

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

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Received: *17 April 2023****, Accepted:*** *22 July 2023*

10.22059/jvr.2023.355694.3329 20.1001.1.20082525.1402.78.3.7.3

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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How to cite this article:

Abolvafaei SZ, Shams N, Forouharmehr A, Jaydari A, Nazifi N. Design and Molecular Docking Study of Recombinant Chimera Protein HBHA-Omp28 for Developing an Efficient Vaccine Against *Salmonella typhimurium*. J Vet Res, 2023; 78(3): 223-233. doi: 10.22059/jvr.2023.355694.3329

Figure Legends and Table Captions