ABSTRACT

Mycobacterium tuberculosis is thriving as a major health problem despite the use of BCG vaccines. There is a dire need to find new vaccine targets in order to control this bacterium. In this study, reverse vaccinology was used to screen hypothetical proteins to find novel protein-based vaccine candidates against *Mycobacterium tuberculosis*. Two hundred ninety seven (297) hypothetical proteins of *Mycobacterium tuberculosis* strain- H37Rv were obtained from NCBI and were analyzed. Twelve of these proteins were predicted to be efficient candidates for the vaccine. These proteins were predicted to have conserved domain, they were used for further analysis. Function prediction was also performed using HHpred and CDD. Physicochemical analysis of selected proteins was performed due to their hypothetical nature. Selected proteins were also presented to both classes of MHC (I and II) using propred I and propred II. All the proteins were bound with several alleles of both classes of MHC (II and II). Virulence analysis was performed using virulentpred which revealed that all the selected proteins were the virulence factor of bacteria. Conservancy analysis was also performed to select the vaccine candidates conserved across most of the strains if not all to overcome the vaccine limitation of associated with serotype specificity. Five out of the twelve proteins; CCP43816.1, CCP44725.1, CCP44726.1, CCP44744.1 and CCP44759.1 were predicted to serve as potential vaccine candidates. Method of peptide-based vaccine candidate identification was also used. A strict criteria of the peptide-based vaccine such as B-cell epitopes prediction and then T-cell epitopes from predicted B-cell epitopes and allergenicity, immunogenicity and TAP binding affinity analysis performed. Good water solubility and other good experimental properties were also checked. Two epitopes conservanacy were finally selected. These two epitopes and 5 proteins possess ideal characteristics such as being extracellular or transmembrane in nature, antigenicity and being non-homologous to human proteins and non-allergic proteins. These peptides and proteins were predicted as probable vaccine candidates to improve existing vaccines to either by replacing existing vaccine or became the part of them.