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Computational Investigation on Protein Sequence of Non-O157 VTEC for Potentiality of Vaccine Production

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***Abstract*—Computational method can be used for investigation of the protein sequences for developing a vaccine against infections. In this present study, a protein derived from non-O157 Verotoxin-producing *E. coli* (VTEC) was identified as a potential vaccine candidate that can be used to evaluate their immunogenicity and protective capability against VTEC infections. Identification of potential B-cell epitopes for promising vaccine was carried out by evaluating the protein derived from non-O157 VTEC with the methods of beta turns, hydropathicity, surface accessibility and antigenicity. The methods were implemented in MATLAB. Our test results demonstrated that the VTEC-derived protein has plausible characteristics which provide significant insights for further investigations and will assist in finding potential drug targets/vaccine candidates.**

Keywords— Modeling, Protein sequencing, Verotoxin-producing E. coli, B-cell epitopes.

I. INTRODUCTION

Prediction and development of novel vaccine candidates by computational simulation approaches for numerous diseases have attained a positive response and greatly aided the molecular synthesis to produce safe and effective vaccines. Diarrhea, one of the diseases, caused by Verotoxin-producing *E. coli* (VTEC) troubles the communities across the world . A virulent group of bacteria called non-O157 VTEC is responsible for mild diarrhoea to severe bloody diarrhoea among the children and infants [1]. Treatment of infections becomes more complicated, and at times, almost unmanageable [2, 3]. In some cases, VTEC infection may lead to kidney failure and seldom death [4]. Virulent factors of non-O157 VTEC are vigorous and change with period and environment [5].

Understanding the molecular epidemiology of VTEC virulent factors is complex due to diversity and dynamic characteristics. Identification of a potential antigenic source to which an antibody binds, could be a key step towards decreasing the prevalence of VTEC pathogen as well as reducing the risk, preventing, or treating infections [6]. In principle, an antigen e.g., verotoxin in the form of a pathogen is neutralized through binding by antibodies produced from white blood cell which is known as B cell.

Efficient therapeutic antibodies and target specific vaccine development require a prediction of potential B-cell epitope which is the part of an antigen, recognized by antibodies generated by B cells [7]. The foremost reason for epitope prediction is to define an antigen in the potential antibody prediction, serological diagnosis and immunization. Prediction of B-cell epitopes plays an essential role in antibody therapeutics, vaccines (peptide-based) and immunological diagnostic tools. Structural and functional epitope mapping methods are time-consuming and expensive and often fail to detect potential epitopes. B-cell epitope prediction tools such as ABCpred, BepiPred, BCPreds and AAP algorithms are frequently used for detection of antigenic portions of protein. However, successful identification and classification of proteins serve the importance of selecting suitable B-cell epitopes. Antigenicity, flexibility, beta-turn, surface accessibility and hydrophobicity are the main parameters to express a discontinuous and conformational B-cell epitope.

At present, there is no effective treatment or prevention for Hemolytic uremic syndrome (HUS) caused by VTEC [8]. This scenario motivated us to determine and classify potential B-cell epitopes by computational approach using different parameters and scales for finding novel immunogens. In this research, a protein sequence derived from non-O157 Verotoxin-producing *E. coli* (VTEC) is examined to find significant insights to discover whether it can be used for a potential vaccine. Besides, B-cell epitopes identification may advance the therapeutics antibody against microbial toxins. Moreover, verotoxin B-cell with a high affinity to the antibody may introduce a new vaccine candidate against VTEC infections.

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