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Epitope order Matters in multi-epitope-based peptide (MEBP) vaccine design: An in silico study

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ABSTRACT

The SARS-CoV-2 global pandemic has caused multiple waves of infection, with severe virulent variants of COVID-19. Current pandemic is becoming more lethal by the day and the world is facing an exponential increase in secondary infections and mortality. There is an urgent need for more efficient and agile methods of vaccine development against SARS-CoV-2. Compared to experimental protocols, the opportunities to innovate are very high in immunoinformatics/in silico approaches, especially with the recent adoption of structural bioinformatics in peptide vaccine design. In recent times, multi-epitope-based peptide vaccine candidates (MEBPVCs) have shown extraordinarily high humoral and cellular responses to immunization. Most of the publications claim that respective reported MEBPVC(s) assembled using a set of in silico predicted epitopes, to be the computationally validated potent vaccine candidate(s) ready for experimental validation. However, in this article, for a given set of predicted epitopes, it is shown that the published MEBPVC is one among the many possible variants and there is high likelihood of finding more potent MEBPVCs than the published candidate. To test the same, a methodology is developed where novel MEBP variants are derived by changing the epitope order of the published MEBPVC. Further, to overcome the limitations of current qualitative methods of assessment of MEBPVC, to enable quantitative comparison, ranking, and the discovery of more potent MEBPVCs, novel predictors, Percent Epitope Accessibility (PEA), Receptor specific MEBP vaccine potency(RMVP), MEBP vaccine potency(MVP) are introduced. The MEBP variants indeed showed varied MVP scores indicating varied immunogenicity. Further, the MEBP variants with IDs, SPVC_446 and SPVC_537, had the highest MVP scores indicating these variants to be more potent MEBPVCs than the published MEBPVC and hence should be prioritized for experimental testing and validation. The computationally validated top-ranked MEBPVCs must be experimentally tested, validated, and verified. The differences and deviations between experimental results and computational predictions provide an opportunity for improving and developing more efficient algorithms and reliable scoring schemes and software.

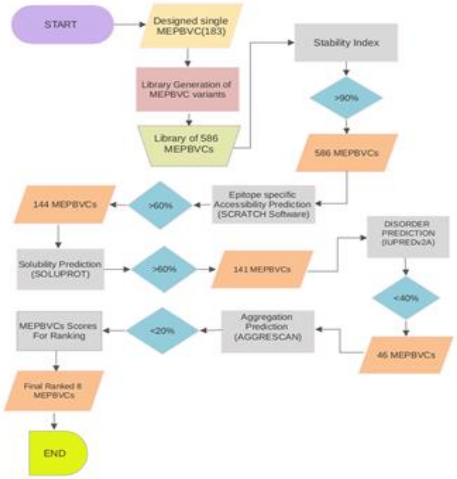

Figure: Schematic workflow for the generation multi-epitope based peptide vaccine

BIOGRAPHY

Burra V L S Prasad has a doctoral degree in Structural Bioinformatics, Protein Crystallography from Molecular Biophysics Unit (MBU), Indian Institute of Science (IISc), Bangalore. He is an engineer by training in Agricultural Engineering and holds a Master's Degree in Biotechnology from School of Life Sciences, University of Hyderabad. He has approximately 23 years of research experience, 5 years of industry experience and 12 years of teaching experience. He has many publications in international journals including PNAS, PLOS-One, JMB, JIB, ACTA-D, Proteins among others. His current focus is design and development of therapeutics and peptide based vaccine design against COVID19, TB and Cancer. He is currently the PI of three extramural funded project grants. Dr. Prasad's research interests include therapeutics, MEBP vaccine design, genomics technologies, bio-tensegrity and biological programming & software. In addition his focus is on bio-algorithms, analysis and automation. He has been an academic administrator heading various lead positions.

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