

***In Silico* Studies of Toxicity, Hydrophobicity, and Hydropathicity on Predicted Epitope of Denv Using Bioinformatics Tools**

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Structured Abstract

Background: Dengue fever is a serious global health issue caused by the dengue virus (DENV), which has four serotypes: DENV-1, DENV-2, DENV-3, and DENV-4. Developing a vaccine is challenging due to the risk of severe infections from different serotypes and a condition called antibody-dependent enhancement (ADE), which if someone gets infected by one type of serotype of the DENV virus, their second infection with another type of serotype can be even more severe.

Methods: This study focuses on using *in silico* bioinformatics tools to predict the toxicity, hydrophobicity and hydropathicity of DENV epitopes to support vaccine development. Two key epitopes, EP12 and EP15, were selected from NS1 protein sequences using data from Abdul Rohim and Kambol (2024). The toxicity of these epitopes was analyzed with ToxinPred (Gupta et al., 2013), while their hydrophobicity and hydropathicity were evaluated using ProtScale (Gasteiger et al., 2005) tools with the Kyte-Doolittle (1982) and Hopp-Woods (1981) scales.

Results: The result shows EP12 is better than EP15 which in the toxicity test, all segments of EP12 have negative SVM scores (-1.52 to -0.66), which are below the toxicity cutoff of 0, while EP15 has some segments with positive scores (0.06), indicating possible toxicity. For hydrophobicity, EP12 has a balanced profile, with slightly hydrophobic regions (score 0.533) with cutoff 0 to +1.0 and no strongly hydrophobic areas. In hydropathicity, EP12 is mostly hydrophilic (score range 0.078 to 0.7), while EP15 has several strongly hydrophobic regions (-1.289), which is not ideal.

Conclusion: Therefore, EP12 is the better candidate for the dengue vaccine, because of non-toxic, having a slightly hydrophobicity (balanced), and showing good hydropathicity. This study successfully demonstrates how bioinformatics tools like ToxinPred (Gupta et al., 2013) and ProtScale (Gasteiger et al., 2005), which include the Kyte-Doolittle (1982) and Hopp-Woods (1981) scales, help identify possible vaccine candidates, making it easier to develop vaccines for which a universal vaccine covering all serotypes is not yet available.

Keywords: Toxicity, Hydrophobicity, Hydropathicity, Support Vector Machine (SVM), Serotypes

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