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Molecular modeling and conformational epitope prediction of nucleocapsid protein region from Japanese encephalitis virus

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The 3D structure of a protein is a prerequisite for structure based drug design as well as for identifying the conformational epitopes that are essential for the designing vaccines.

A 3-dimensional model (3D) was developed for the nucleocapsid protein of Japanese encephalitis virus. A homology modeling method was used for the prediction of the structure. For the modeling, one template proteins were obtained by mGenTHERADER, namely the high-resolution X-ray crystallography structure of NS3 protease helicase of murry vally encephalitis virus(2WV9). By comparing the template protein a rough model was constructed for the target protein using SWISSMODEL, a program for comparative modelling. The model was validated using protein structure checking tools such as Verify3D and Anola for reliability. The total of 138 such epitope regions/sites have been identified by kolaskar and tongaokar method. Conformational epitopes are mapped from the 3D structure of nucleocapsid protein of Japanese encephalitis virus modeled using the concept of an antigenic domain. The information thus discussed provides insight to the molecular understanding of nucleocapsid protein of JE virus. The predicted 3-D model may be further used in characterizing the protein in wet laboratory.

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