

HPV-16, HPV-11 AND HPV-06 E1 DNA BINDING DOMAIN PROTEIN MODELLING BY HOMOLOGY

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The Human Papillomavirus (HPV) is a DNA virus family associated with cervical cancer (HPV-16 and 18) and benign mucosal lesions (HPV-6 and 11), represented by more than 200 types of different genotypes. Interactions between DNA-Binding Domain (DBD) E1 Protein and Replication Origin allow the beginning of the viral replication process. Molecular Modeling by Homology is based on the principle that amino acid (AA) homology sequences have structural and functional similarity. This is useful to suggest the three-dimensional protein structure that does not have a crystallographic structure. In this study, we propose a model for E1 Protein DBDs region of HPV-16, 11 and 6, based on MMH using BPV-1 and HPV-18 crystallographic structures as model since significant homology. To build the models we used the Swiss-Pdb Viewer. Then, the model was submitted to the SWISS-MODEL server to validate an initial model. The Ramachandran plot shows only one residue in the unfavorable regions for the HPVs. We analyzed the secondary structure properties and the interactions among important AAs to E1 DNA binding, described in the literature. Some differences as high hydrophobicity AAs and secondary structural changes in these regions suggest some variation in E1 DBD for high and low-risk HPV types.

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