Computational Prediction of Vaccine Potential Epitopes and 3D Structure of XAGE-1b for Non-small Cell Lung Cancer Immunotherapy

Mansour, Mohamed

XAGE-1b is highly and strongly expressed in lung adenocarcinoma and immunogenic in patients, regarded as one of the most immunogenic antigens. In this in silico study, I worked on predicting the best antigenic determinants from 9 KD Cancer /testis XAGE-1b.Using computer tools and trusted databases, antigenicity prediction plots were generated showing most antigenic segments. I performed computational prediction for T cell CD8 epitopes peptides proposing XAGE-1b(57-65) to be an HLA-A*11:01-restricted nonamer as the highest binding score peptide and XAGE-1b(30,38) as an HLA-A*02:06-restricted 9-mer peptide which has the highest binding score. T cell CD4 prediction results analysis suggested XAGE-1b(33-47) to be an HLA-DRB1*0405-restricted 15-mer peptide as the highest score and the lowest percentile rank peptide as well as XAGE-1b(54-68) peptide to be a DRB1*0410-restricted 15-mer peptide, the predicted peptides showed higher scores than experimentally identified peptides to the same alleles. Despite its importance in Cancer research, the 3D structure of this protein is not available and its confirmation hasn’t been solved experimentally yet. I ran multiple sequence alignment to select most reliable modeling templates and homology modeling technique was performed using computer-based tool to generate 3D structure models. For the verification of the predicted models different validation tools were used showing a good quality model. The contributions of this study can be very useful for demonstrating the tertiary structure of XAGE-1b which helps us to determine it's function and using the suggested peptides for epitope vaccine designing and development against NSCLC.