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In silico Epitope Mining and the Search for a Universal Carrier Protein

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Vaccines against drugs of abuse (VADAs) have long been of interest as a possible therapeutic for the alleviation of addiction. These vaccines, however, have failed in many clinical trials due to extensive variability in antibody response between individual subjects. Correspondingly, the future success of VADAs hinges directly on whether or more broadly effective vaccines can be engineered. Differences in response must, to some extent, be the result of variable capacities for each individual's immune system to process and/or present antigen. As such, future VADAs will need to find ways to rationally potentiate antigen processing / presentation in the majority of subjects based on quantifiable properties of the target population. Here, we describe the initial tasks of a project aiming to engineer a broadly effective carrier protein. Using haplotype frequency data provided by Be the Match, HLA-DQ haplotypes covering 99% of the population were selected for analysis (15 beta chains, 420 alpha-beta pairs). Next, the most common carrier proteins used in conjugate vaccine formulations were analyzed for MHC II epitope content using the selected HLA-DQ alleles and NetMHCIIpan 3.2 prediction software. Finally, we used a modified version of the prediction output to excise the most likely MHC II epitopes from the analyzed proteins based on the mean, standard deviation, and anchor residue likelihood values of amino acids when all predictions for a protein were combined. These results present the successful first steps for the construction of an *in silico* derived, broadly effective carrier protein to be used in future VADA formulations.