NetMHCIIpan-3.0, a common pan-specific MHC class II prediction method including all three human MHC class II isotypes, HLA-DR, HLA-DP and HLA-DQ

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Major histocompatibility complex class II (MHCII) molecules play an important role in cell-mediated immunity. They present specific peptides derived from endosomal proteins for recognition by T helper cells. The identification of peptides that bind to MHCII molecules is therefore of great importance for understanding the nature of immune responses and identifying T cell epitopes for the design of new vaccines and immunotherapies. Given the large number of MHC variants, and the costly experimental procedures needed to evaluate individual peptide–MHC interactions, computational predictions have become particularly attractive as first-line methods in epitope discovery. However, only a few so-called pan-specific prediction methods capable of predicting binding to any MHC molecule with known protein sequence are currently available, and all of them are limited to HLA-DR. Here, we present the first pan-specific method capable of predicting peptide binding to any HLA class II molecule with a defined protein sequence. The method employs a strategy common for HLA-DR, HLA-DP and HLA-DQ molecules to define the peptide-binding MHC environment in terms of a pseudo sequence. This strategy allows the inclusion of new molecules even from other species. The method was evaluated in several benchmarks and demonstrates a significant improvement over molecule-specific methods as well as the ability to predict peptide binding of previously uncharacterised MHCII molecules. To the best of our knowledge, the NetMHCIIpan-3.0 method is the first pan-specific predictor covering all HLA class II molecules with known sequences including HLA-DR, HLA-DP, and HLA-DQ. The NetMHCpan-3.0 method is available at http://www.cbs.dtu.dk/services/NetMHCIIpan-3.0.

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